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Relativistic Theory of Atoms and Molecules III

Pekka Pyykkö

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Preface

Seven years have elapsed since "RTAM II" was published in 1993. Together with "RTAM I", published in 1986, it contained 6577 references. The present volume covers the years 1993-99. The running numbers in the present volume begin from 6578 and end at 10369. Gradually, the present volumes seem to be forming a *Köchel-Verzeichnis* of relativistic calculations on atoms and molecules. In the present volume, a certain degree of completeness on molecular production work was still attempted, although certainly not reached. In the future that would be both more and more difficult and less and less meaningful.

The molecular production work using all methods is now collected to the single Table 7.10 and ordered by the element, or group of elements, considered characteristic. This will facilitate the comparisons between different methods.

The data base corresponding to the latter part of the book will be made available in the World Wide Web at *http://www.csc.fi/lul/rtam*. The analysis in the tables is not available in the Web.

I thank the *Royal Society of Chemistry* and my coauthor *Herman Stoll* for permission to include in the present Table 7.10 material from my review on pseudopotential calculations in *Royal Society Periodical Reports, Chemical Modelling, Applications and Theory (2000)*.

I apologise for any inadvertent omissions or characterisations that the author would not find fitting. No legal responsibility is accepted in such cases.

I thank *Jonas Jusélius* for technical advice and The Academy of Finland for a Research Professorship in August 1995–July 2000. I also thank the Springer-Verlag for constructive cooperation during the past years.

Helsinki, 31 October, 2000

Pekka Pyykkö

Contents

List of Tables

Chapter 1

Introduction

Table 1.1. gives a list of treatises and other general references. For a list of symbols and acronyms, see the end of the book.

Table 1.1: Monographs, reviews and other general references.

Reference	Comments
Kessler (1985)	Polarized electrons.
Lindgren and Morrison (1986)	Atomic many-body theory.
Benn and Tucker (1988)	Introduction to spinors.
Ryder (1988)	Text on quantum field theory. New derivation of Dirac equation.
Akai et al. (1990)	Theory of hyperfine interactions in metals.
Lindgren (1992,1994)	Reviews on the atomic many-body problem.
Yarkony (1992)	Spin-forbidden chemistry within BP approximation. Review.
T.-N. Chang (1993)	MBPT of atomic structure and photoionization.
Drake (1993ab)	High-precision calculations and QED effects for 2- and 3-electron atoms.
Drake (1993c)	He Rydberg levels.
Fanchi (1993)	Parametrized relativistic quantum theory. Book.
F. Gross (1993)	Relativistic quantum mechanics and field theory. Book.
Johansson and Brooks (1993)	Theory of cohesion in lanthanides and actinides.
Johnson (1993)	Relativistic MBPT on highly-charged ions.
Y.-K. Kim (1993ab)	Recent and unsettled questions in atomic structure theory.
Labzowsky et al. (1993b)	Treatise on relativistic and QED effects in atoms.
Levin and Micha (1993)	Long-range Casimir forces. Book.
Lindgren et al. (1993a)	Heavy ion spectroscopy and QED in atomic systems.
Mårtensson-Pendrill (1993a)	MBPT in atomic structure calculations.
Mårtensson-Pendrill (1993b)	PNC effects in atomic systems.
Minaev and Lunell (1993); Minaev (1996); Minaev and Ågren (1995,1996)	SO effects in organic reactions.
Mohr (1993,1994)	QED in few-electron systems.
Norman and Koelling (1993)	Electronic structure of f electron metals.
Sandars (1993)	P and/or T violation. Review.
Sapirstein (1993)	Theory of many-electron atoms. Review on QED and many-body aspects.
Adler (1994)	Quaternionic QM and quantum fields.
Altmann and Herzig (1994)	Comprehensive point-group theory tables.
Balasubramanian (1994)	Lanthanide and actinide molecules.
Dyall (1994c)	Review on DF/GTO for polyatomic molecules.
Ermler and Marino (1994,1996)	Reviews on PP methods.
Froese Fischer and Jönsson (1994)	Review on MCHF atomic calculations.
Grant (1994ab,1996)	Reviews on relativistic atomic calculations.
Greiner (1994,1997)	Relativistic quantum mechanics. Wave equations. Book.
Malli (1994ab)	Relativistic and electron correlation effects in molecules and solids.
Marian (1994)	Relativistic calculations on transition metal compounds.
Schweber (1994)	History of QED.
Bauschlicher et al. (1995)	Transition-metal compounds.
Borovskii et al. (1995)	Plasma of multicharged ions.
Eichler and Meyerhof (1995)	Relativistic atomic collisions.

Reference	Comments
Engel (1995); Engel and and Dreizler (1996)	Relativistic density functional theory.
Hess et al. (1995)	Review on SO effects and methods.
Kaldor (1995,1997)	Reviews on the Fock-space CC approach.
Lindgren et al. (1995b)	Few-body problems in atomic physics.
Porteous (1995)	Clifford algebras and classical groups.
Robinson (1995)	Textbook on special relativity.
Schädel (1995)	Chemistry of transactinides.
Ågren et al. (1996)	SO phenomena in molecules. Handled with response theory.
Aksela et al. (1996a)	Resonant and nonresonant Auger recombination.
Almlöf and Gropen (1996)	Relativistic effects in chemistry.
Cundari et al. (1996)	Review on PP methods.
Dolg and Stoll (1996)	Review on lanthanide chemistry.
Ebert (1996)	Magneto-optical effects in TM systems.
Ebert and Schütz (1996)	SO-influenced spectroscopies of magnetic solids.
Frenking et al. (1996,1999); Frenking and Pidun (1997)	Transition-metal compounds. Especially PP work.
Gordon and Cundari (1996)	PP studies on transition-metal compounds. Review.
E. K. U. Gross et al. (1996)	DFT of time-dependent phenomena.
Labzowsky (1996)	Treatise on QED of atoms.
Lindgren (1996)	Relativistic many-body and QED calculations on atomic systems.
Mohr (1996)	Tests of fundamental physics.
Musaev and Morokuma (1996)	Potential-energy surfaces of TM-catalyzed chemical reactions.
Pachucki et al. (1996)	Theory of energy levels and precise two-photon spectroscopy of H and D.
Pershina (1996)	Electronic structure and properties of transactinides and their compounds.
Roos et al. (1996)	Review multiconfiguration PT for molecules. Includes PT relativity.
Rösch et al. (1996)	Review on DK DFT molecular calculations.
Sapirstein (1996a)	Quantum electrodynamics.
Siegbahn (1996)	Electronic structure calculations for molecules containing transition metals.
van der Lugt (1996)	Polyanions, especially Zintl anions, in ionic alloys A review.
Yndurain (1996)	Relativistic QM. Book.
Andersen et al. (1997)	Negative alkaline-earth ions.
Baerends and Gritsenko (1997)	Quantum chemical view on density-functional theory.
Balasubramanian (1997a)	Relativistic quantum chemistry: methods.
Balasubramanian (1997b)	Relativistic quantum chemistry: applications.
Bouchiat and Bouchiat (1997)	Review on parity violation in atoms.
Edmonds (1997)	Book on relativity.
Ehlotzky et al. (1997)	Review on electron-atom collisions in laser fields.
Fricke et al. (1997)	Review on superheavy elements as treated by DFT-DVM.
Hess (1997)	Review on relativistic effects in heavy-element chemistry.
Kaltsoyannis (1997a)	Relativistic effects in inorganic and organometallic chemistry.
Y.-K. Kim (1997)	Review on relativistic atomic structure calculations.

Reference	Comments
Mohr (1997)	QED corrections in heavy atoms.
Persson et al. (1997b)	Theoretical survey of QED tests in highly charged ions.
Pyykkö (1997)	Strong closed-shell interactions in inorganic chemistry.
Rudzikas (1997)	Theoretical atomic spectroscopy.
Schädel et al. (1997ab)	Experimental chemistry of Sg (E106).
Schwabl (1997)	Advanced QM. Book. Dirac equation, QED.
Snygg (1997)	Book on Clifford algebra.
Stöcker et al. (1997)	Structure of vacuum and elementary matter. Conference proceedings.
Tomonaga (1997)	History of spin.
Dolg (1998)	Lanthanides and actinides.
Dzuba et al. (1998)	Atomic MBPT.
Godefroid et al. (1998)	Review on atomic structure calculations.
Grabo et al. (1998)	Optimized effective potential DFT. Review.
Hess (1998)	Review on relativistic theory and applications in chemistry.
Lindgren (1998)	Electron correlation and QED.
I. Martin (1998)	Relativistic quantum defect orbital method.
Nemoshkalenko and Antonov (1998)	Computational methods in solid-state physics.
Sapirstein (1998)	Theory of many-electron atoms. Review on QED and many-body aspects.
Schwerdtfeger and Seth (1998)	Relativistic effects in superheavy elements.
Shabaev et al. (1998c)	QED and nuclear effects in highly charged ions.
Soff et al. (1998)	QED in strong fields. Review.
Strange (1998)	Relativistic QM with condensed-matter and atomic physics applications. Book.
Datz et al. (1999)	Atomic physics. Review.
Ellis and Guenzburger (1999)	Review on the Discrete Variational Method in DFT.
Fröhlich and Frenking (1999)	Bonding in transition-metal complexes. Carbonyls, carbenes, π-bonded systems, dihydrogen complexes.
Greiner and Gupta (1999)	Edited book on superheavy elements.
Kaldor and Eliav (1999)	High-accuracy calculations for heavy and superheavy elements.
Kleppner (1999)	Atomic physics in the 20th century.
Lindgren (1999)	QED effects in strong nuclear fields.
Pershina and Fricke (1999)	Electronic structure and chemistry of the heaviest elements.
Pettersson et al. (1999b)	New rare-gas-containing neutral molecules. Review.
Quiney et al. (1999)	Ab initio relativistic quantum chemistry.

Chapter 2

One-Particle Problems

Table 2.1: The Dirac equation: historical notes, interpretative studies, symmetry properties and non-relativistic limits.

Reference	Comments
Takabayasi (1955)	Structure of Dirac wave function.
Takabayasi and Vigier (1957)	Relativistic hydrodynamics of Dirac matter.
Gorshkov (1962)	Scattering of Dirac particle from Coulomb field with finite-nucleus and screening corrections.
Barut (1973)	Extensions of Dirac Hamiltonian using Lie algebra.
Triebel (1980)	Dirac operators. Textbook of higher analysis.
Ryder (1988)	Alternative derivation of Dirac equation starting from plane waves.
Briegel et al. (1991)	Square root of the KG equation.
Aldaya et al. (1993)	Poincaré group and the position operator.
Anandan and Mazur (1993)	Geometric phase for the KG equation.
Avery et al. (1993)	Four-currents in Dirac theory.
Barut (1993)	On 'new constants of motion' for free Dirac electron.
Barut and Cruz (1993)	Classical spinning particle with anomalous magnetic moment.
Barut and Unal (1993)	Poisson brackets and symplectic structures for classical and quantum Zitterbewegung.
Bechler (1993)	Summation formulae for spherical spinors.
Bednar and Kolar (1993)	Relativistic spin projection operators.
Bohm (1993)	R and NR dynamical groups.
Comay (1993)	Interpretation of the Lorentz-Dirac equation.
Corben (1993)	Factors of 2 in magnetic moment, SO coupling, Thomas precession.
Faisal and Radożycki (1993)	Bound KG particle in an intense laser field. 3D model.
Frisk and Guhr (1993)	SO coupling in the semiclassical (WKB) approximation.
Frochaux (1993abc)	Relativistic corrections to Schrödinger equation from quantum field theory.
Hestenes (1993)	Zitterbewegung modelling.
Ito (1993)	Renormalization of relativistic wave function at origin.
Kowalski (1993)	Relativistic nature of the Schrödinger equation. Only one free-particle phase velocity is meaningful.
Lämmerzahl (1993,1994)	Pseudodifferential operator square root of the KG equation.
Lounesto (1993)	Clifford algebras and Hestenes spinors.
Mocanu et al. (1993)	On Thomas rotation paradox.
Okolowski and Slomiana (1993)	R aspects of NR QM. Comment on Dieks and Nienhuis (1990)[4035].
Ord and McKeon (1993)	Feynman chessboard model and the (3+1)D Dirac equation.
Pauri (1993)	Constants of motion for free Dirac particle.
Pavšič et al. (1993)	Classical models for spin.
Pilkuhn and Staudner (1993)	Double Dirac equation and decay rates of bound particles.
Rodrigues et al. (1993)	Zitterbewegung and electron structure.
Shin and Rafelski (1993)	Relativistic classical ($\hbar \to 0$) limit of quantum theory.
Vaz and Rodriguez (1993)	Zitterbewegung and the EM field of the electron.
Y. X. Zheng (1993)	Regularity of weak solutions to a 2D modified Dirac-KG equation.
Aliev et al. (1994)	Path-integral representation for Dirac propagator.
Barut (1994)	Localized mass-less wavelets with half-integer spin.
Barut and Cruz (1994)	The Zitterbewegung of the relativistic electron. Comments on Sherry (1988).

Reference	Comments
Barut and Pavsic (1994)	Dirac's shell model of the electron. Moving relativistic charged membranes.
Z. Chen et al. (1994)	Upper and lower bounds for 1-electron Dirac Hamiltonian. Tests on Coulomb potential.
Forte (1994)	Relativistic quantum theory with fractional spin and statistics.
Greiner (1994,1997)	Relativistic quantum mechanics. Wave equations. Book.
Grosse et al. (1994)	Order and spacings of KG energy levels.
Hill and Krauthauser (1994)	Variational collapse avoided by using $1/h_{\rm D}$ instead of $h_{\rm D}$. Application on the H atom.
Land et al. (1994)	Selection rules for dipole radiation from a relativistic bound state.
Pillin (1994)	q-deformed relativistic wave equations.
Rivas (1994)	Dirac equation obtained by quantizing a classical spinning particle.
Shankar and Mathur (1994)	Thomas precession, Berry potential and the 'meron'.
Vrbik (1994)	Dirac equation and Clifford algebra.
Waxman (1994)	Fredholm determinant for Dirac operator. 1D, some $V(x)$. Periodic boundary conditions.
Aldaya and Guerrero (1995)	A finite enlargement of the (1+1)D Poincaré group. Boost $i\frac{\partial}{\partial \pi}$.
Aparicio et al. (1995)	Feynman parametrization of the Dirac equation.
Augenstein (1995)	Quotes Y. Frenkel [Z. Phys. 47 (1928) 786] and D. Iwanenko and L. Landau [Z. Phys. 48 (1928) 340] as precursors for the Dirac equation.
Baylis and Sienkiewicz (1995)	Represent electron-scattering polarization data by 'polarization trajectories' on a Poincaré sphere.
Blancarte et al. (1995)	High- and low-energy estimates for the Dirac equation. Levinson theorem for the zero-mass limit.
Caspersson (1995)	Dirac equation at semiclassical limit.
Cooper et al. (1995)	Supersymmetry and the Dirac equation. Coulomb and Lorentz scalar potentials. Magnetic field.
Gaioli and Garcia Alvarez (1995)	Intrinsic parity in Ryder's (1988) derivation of the Dirac equation.
Jefimenko (1995)	Retardation and relativity for a moving line charge.
Land and Horwitz (1995)	Zeeman effect for a relativistic bound state. Zeeman splitting in manifestly covariant form.
Ochs and Sorg (1995)	Relativistic Schrödinger equations and the particle-wave duality.
Petráš (1995)	The $SO(3,3)$ group as common basis for the Dirac and Proca equations.
Phatak et al. (1995)	Semiclassical features of Dirac particle in cavity.
Pilkuhn (1995)	An M1 hyperfine operator between two Dirac particles, both having anomalous magnetic moments.
Boeyens and Kassman (1996)	Introduction of spin into the Schrödinger equation.
Crisp (1996)	Relativistic neoclassical radiation theory.
De Leo (1996)	Quaternions and special relativity.
Goodmanson (1996)	A graphical representation of the Dirac algebra.
Hamilton (1996)	Relativistic precession.
Jefimenko (1996)	Relativistic force transformation from Lorentz force law.
Lerner (1996)	Derive Dirac equation from relativistic representation of spin.
Ord (1996)	Relationships between the Schrödinger and Dirac equations and the random walk Brownian motion formalism of diffusion.

Reference	Comments
Oudet (1996)	Discusses interpretation of g-factors and spin.
Philpott (1996)	Thomas precession and the Liénard-Wiechert field.
Robson and Staudte (1996)	An eight-component relativistic wave equation for spin-$\frac{1}{2}$ particles. Solved for the H atom.
Salcedo and Ruiz Arriola (1996)	Wigner transformation for the determinant of Dirac operators.
Zhuang and Heinz (1996)	Kinetic equations for Dirac particle with EM, scalar, and pseudoscalar interactions.
Booth and Radford (1997)	Dirac-Maxwell equations with cylindrical symmetry.
Dahl (1997)	Physical origin of Runge-Lenz vector.
Gitman and Shelepin (1997)	Poincaré group and relativistic wave equations in 2+1 dimensions. Anyons, with any spin and statistics.
Gomes et al. (1997)	Relativistic corrections to Aharonov-Bohm scattering.
Y. S. Huang et al. (1997)	Alternative to KG for spin-0 particles.
Isozaki (1997)	Inverse scattering theory for Dirac operators.
Jung (1997)	Geometrical approach to inverse scattering for Dirac equation.
Nakamura (1997)	Path space measures for Dirac and Schrödinger equations.
Omnès (1997)	Localization of relativistic particles.
Pelc and Horwitz (1997)	Complete sets of states in relativistic scattering theory.
Zakrzewski (1997)	Localization of relativistic systems.
Bechouche et al. (1998)	NR limit of the Dirac equation for time-dependent EM fields.
Bolte and Keppeler (1998, 1999)	Semiclassical time evolution of R spin-$\frac{1}{2}$ particles. Dirac equation at the limit $\hbar \to 0$.
Breuer and Petruccione (1998)	Quantum-state diffusion for a Dirac electron.
Cohen and Leung (1998)	Relativistic corrections to atomic sum rules.
S.-H. Dong et al. (1998)	Relativistic Levinson theorem in 2D.
Finster (1998)	Local $U(2,2)$ symmetry in relativistic quantum mechanics.
Gosselin and Polonyi (1998)	Path integral for relativistic equations of motion. KG and Dirac.
Popov et al. (1998)	Relativistic version of the imaginary time method. Applications on ionization.
Reginatto (1998)	Derives the Pauli equation using the principle of minimum Fisher information.
Ruijgrok (1998)	General requirements for a relativistic quantum theory.
Ryder (1998)	Relativistic spin operator for Dirac particles.
Sharma et al. (1998)	NR limit for particle of arbitrary spin in external field.
Unterberger (1998)	A calculus of observables on a Dirac particle.
K. Ziegler (1998)	Delocalization of 2D Dirac fermions with random mass. Role of broken supersymmetry.
Avetissian et al. (1999)	Eikonal wave function for Dirac particle in arbitrary potential and radiation fields.
Baylis and Yao (1999)	Relativistic dynamics of charges in EM fields using eigenspinors.
Bohm and Kaldass (1999)	Relativistic partial-wave analysis using the velocity basis of the Poincaré group.
Boya and Byrd (1999)	Clifford periodicity from finite groups.
Bracken and Melloy (1999)	Localizing the relativistic electron. Free electron 4-vector density $(\rho(x,t), j(x,t)/c)$ can be localized using only positive-energy states.
des Cloizeaux (1999)	Dirac equation formulated in terms of local observables.

Reference	Comments
S.-H. Dong et al. (1999)	Levinson theorem for the KG equation in 2D.
Edmonds (1999)	Dirac's equation in half of his algebra.
García-Calderón et al. (1999)	Low-energy relativistic effects in discussing time-dependent tunneling.
Jaekel and Reynaud (1999)	Observable Dirac electron in accelerated frames. Localization observables.
Mattes and Sorg (1999a)	Second-order mixtures in relativistic Schrödinger theory.
Mattes and Sorg (1999b)	Two-particle systems with EM interactions in relativistic Schrödinger theory.
Pissondes (1999)	Recovers the KG equation in 'scale-relativity theory'.
Şimşek (1999)	Negative-energy levels for a ND Dirac equation. Spherically symmetrical, purely imaginary, linear potential.
Tkachuk and Roy (1999)	Supersymmetry of a spin-$\frac{1}{2}$ particle on the real line. Rotating magnetic field + a scalar potential.
B.-X. Wang and Lange (1999)	Attractors for the KG equation.
Z.-C. Wang and Li (1999)	Geometric phase in Dirac theory. (Cp. Berry). Lorentz invariant.

The Table 2.2 below discusses transformations of the Dirac equation. For further examples from quantum chemical calculations, see also the Table 7.3.

Table 2.2: The Dirac equation: further transformations.

Reference	Comments
Fraga and Karwowski (1974)	Two nuclear-mass-dependent terms in the BP equation. Of same order as the hyperfine interaction.
Arriola and Salcedo (1993)	Semiclassical expansion of Dirac Hamiltonians.
Mustafa and Sever (1993)	Shifted $1/N$ expansion for a relativistic spin-$\frac{1}{2}$ particle.
Q.-S. Wang and Stedman (1993)	Derives from FW an E1 term of form $qs \cdot \dot{\mathbf{A}} \times \mathbf{p}/2m^2c^2$. Applications to lanthanides.
Faulkner (1994)	Scattering matrices for non-spherical SR potential.
Fearing et al. (1994)	Compare the FW and Pauli approximations in nuclear physics. FW found better.
Aucar et al (1995b)	Bethe sum rule for the no-pair Hamiltonian.
Costella and McKellar (1995)	The FW transformation.
Grigoryan and Grigoryan (1995)	Quasiclassical FW transformation and canonical quantization of $D = 2n$-dimensional relativistic particles in external EM field.
Lucha and Schöberl (1995)	Semirelativistic Hamiltonians of apparently nonrelativistic form. Effective mass
van Lenthe et al. (1995)	Solves the 2nd-order Dirac equation for the large component in a Slater basis. Tests on U atom.
Amore et al. (1996)	Effective potentials for nuclear physics via FW.
Ebert et al. (1996);	SO effects for Dirac equation and spin-dependent potentials
Guil and Mañas (1996)	The 2D heat equation yields the KG equation, which is here expressed in terms of solutions of the Dirac equation. KD = Kadomtsev-Petiashvili equations.
Lévai and Del Sol Mesa (1996)	Transform the Dirac equation into a Schrödinger-like one for minimal and non-minimal couplings. Polynomial potentials.
Ebert et al. (1996);	SO effects for Dirac equation and spin-dependent potentials

Reference	Comments
Ebert et al. (1997b)	divided into two parts, diagonal and off-diagonal.
Staudte (1996)	An eight-component wave equation for spin-$\frac{1}{2}$ particles. Part II.
van Lenthe et al. (1996a)	Solve the Dirac equation using the FW transformation and large components only. Tests on U atom.
Dyall (1997)	'Normalized elimination of small components'.
Lagmago Kamta et al. (1998)	Semiclassical KG dipole matrix elements.
Nikitin (1998)	New classes of external fields having an exact FW transformation.
Kocinski (1999)	A 5-dimensional form of the Dirac equation. Pauli limit derived.
Nowakowski (1999)	QM current of Pauli equation.

Table 2.3: The Dirac equation: solutions for hydrogen-like systems.

Reference	Comments
Gorshkov (1962)	Scattering of Dirac particle from Coulomb field with finite-nucleus and screening corrections.
Barut and Bornzin (1971)	$SO(4,2)$-Formulation for Dirac and KG equations. With or without magnetic charges.
Tzara (1985)	KG Coulomb problem in momentum space.
Moss and Sadler (1986)	Electric quadrupole moments of one-electron atoms. In $j = \frac{1}{2}$ states due to hfs. Resolves earlier inconsistencies.
Hofstetter et al. (1992)	Ionization of hydrogen by relativistic heavy projectile.
Biedenharn et al. (1993)	Dirac-Coulomb problem and κ-Poincaré group.
Bleyer (1993)	Coulomb problem for generalized Dirac equation.
Bondarev and Kuten (1993)	Polarizability tensors for H-like $ns_{1/2}$ and $np_{1/2}$ states. Due to M1 hfs.
Choe et al. (1993)	Tests of B-spline basis sets on H-like O and Hg.
Cohen and Kuharetz (1993)	DC wave function in Whittaker form. Further solutions to the Darwin-Gordon (1928) ones are presented.
Guiasu and Koniuk (1993)	Particle interpretation of the DC solutions. Effective 'no-pair' one-electron solution found, starting from Fock space.
C. Hofmann et al. (1993)	Distorted-wave scattering solution of Dirac electron from a Coulomb potential.
Horwitz (1993)	Dynamical group of the relativistic Kepler problem. $SO(4,1)$ for the bound states.
Kwato Njock et al.(1993)	E1 radial integrals in semiclassical Coulomb approximation.
Papp (1993)	Dirac-Coulomb and linear potentials using 'β functions'.
Pisani et al. (1993)	Discuss relativistic effects in atoms and molecules using LCAO calculations on H-like systems as example.
Tangerman and Tjon (1993)	Exact supersymmetry in NR H-atom. Pauli particle in Coulomb field.
Yao and Chu (1993)	Pseudospectral methods for bound and resonance state problems with the Dirac equation. H-like atom as example.
Anthony and Sebastian (1994)	Rel. corrections to g-factors of H-like atoms and positronium.
Z. Chen et al. (1994)	Upper and lower bounds for 1-electron Dirac Hamiltonian. Tests on Coulomb potential.
Hill and Krauthauser (1994)	Variational collapse avoided by using $1/h_{\mathrm{D}}$ instead of h_{D}. Application on the H atom.
Kwato Njock et al. (1994a)	Supersymmetry-based QDT of Dirac equation for central potentials.
Le et al. (1994)	DC Green function. Polarizability of H-like atoms.

Reference	Comments
Lucha and Schöberl (1994)	Variational approach to spinless relativistic Coulomb problem.
Melić (1994)	Hydrogenic atom with spinless nucleus in magnetic field.
Norbury et al. (1994)	Exact numerical solution of spinless Salpeter equation in momentum space for Coulomb potential.
Salamin (1994)	Expectation values $\langle nl\|r^{\beta}\|nl\rangle$ with DC wave functions.
Shabaev (1994a)	M1 and E2 hfs of H-like ions. Finite-nucleus corrections.
Talman (1994)	Spurious solutions in matrix approximations to the DC problem.
Tong et al. (1994a)	Relativistic effect on atomic radiative processes. A 'zero' of the H-like E1 transition matrix element found.
van Leeuwen et al. (1994)	ZORA solutions for H-like atoms are scaled Dirac ones. Also ZORA KG.
Baltz (1995)	Coulomb potential from a particle in uniform ultrarelativistic motion.
Baluja (1995)	Dipole polarizability of H-like ions.
Dahl and Jørgensen (1995)	Johnson-Lippmann operator, supersymmetry, normal-mode representations.
Deco et al. (1995)	Scattering involving Coulomb potentials. Ion-atom collisions.
Horbatsch and Shapoval (1995a)	KG Coulomb problem in the Feshbach-Villars representation.
Horbatsch and Shapoval (1995b)	Relativistic two-particle scattering resonances in the Tamm-Dancoff approximation.
Horbatsch and Shapoval (1995c)	Analysis of the DC problem using momentum-space free-particle functions.
Indelicato and Mohr (1995)	Asymptotic expansion of the DC radial Green function.
Le Yaouanc et al. (1995)	High-order expansion of eigenvalues of a relativistic Coulomb equation.
Nag and Roychoudhury (1995)	$1/N$ solution of the DC equation.
Rosenberg (1995)	Electron scattering by heavy hydrogenic ion.
Shabaev et al. (1995)	Hfs of H-like ions.
Kołakowska (1996)	Minimax principle for the DC problem. Spurious roots eliminated, no upper bounds obtained.
Le et al. (1996)	Dynamic polarizability of H-like atoms.
Lucha and Schöberl (1997)	Analytical upper bounds on energy levels of the spinless relativistic Coulomb problem.
Molzberger and Schwarz (1996)	Effects of different order in α^2 on energies of H-like atoms. Compare Dirac with 1st- and 2nd-order DK.
Robson and Staudte (1996)	An eight-component relativistic wave equation for spin-$\frac{1}{2}$ particles. Solved for the H atom.
Villalba (1996)	The DC problem. Solution of Cohen and Kuharetz (1993) for $119 < Z < 137$ unphysical.
Andrae (1997)	Recursive formulae for $\langle r^k\rangle$, $-6 \leq k \leq 5$. Numerical values for $Z = 1$, 80, 137.
Barysz (1997)	Compares Pauli PT, DPT and Dirac levels for H-like systems.
Goodman and Ignjatović (1997)	A simpler solution for the DC problem.
Hylton and Snyderman (1997)	Analytic basis set for high-Z atomic QED. He-like ions. Sturmian DC functions.
Manakov and Zapriagaev (1997)	DC problem by 2nd-order Dirac equation approach. Green functions given.

Reference	Comments
Moiseiwitsch (1997)	Virial theorem for electron capture from H-like atom.
Pyykkö and Seth (1997)	H-like relativistic correction factors for nuclear quadrupole coupling. Analytical solution.
Sergheyev (1997)	Relativistic Coulomb problem for modified Stueckelberg equation.
Shabaev et al. (1997b)	Ground-state M1 hfs splitting of H-like ions. Z=49-83.
Simulik (1997)	Hydrogen spectrum in classical electrodynamics.
Stahlhofen (1997)	Algebraic solutions of DC problems. Symmetries. Relations with Dirac oscillators.
Staruszkiewicz (1997)	The DC problem. The role of the classical Coulomb field.
Szmytkowski (1997)	DC Sturmians and the DC Green function. Relativistic polarizability of the H-like atom, Z=1-137.
Szymanowski et al. (1997)	Two-photon bound-bound amplitudes in H-like atoms. Uses DC Green function in a Sturmian basis.
Zolotorev and Budker (1997,1999)	PNC in relativistic hydrogenic ions. Circular dichroism on the $1s \rightarrow 2s$ transition due to interference between the M1 and PNC-induced E1 amplitudes.
Al-Jaber (1998)	N-dimensional hydrogen atom at BP level.
J.-J. Chang (1998)	Similarities between Dirac-Coulomb and Schrödinger-Coulomb radial functions. Photoionization of H.
Dragić et al. (1998)	H atom with added magnetic SO and spin-spin interactions. No deep-lying extra levels found.
Eichler et al. (1998)	Alignment caused by photoionization and in radiative electron capture into excited states of high-Z H-like ions.
Indelicato and Mohr (1998a)	Coordinate-space approach to bound-electron SE. Coulomb-field calculation.
Martínez-y-Romero et al. (1998,1999)	Non-unitary $SU(2)$ representations in a Dirac H atom.
Matrasulov (1998,1999)	Chaotic ionization of an H-like atom in intensive monochromatic field.
Pivovarov (1998)	Coherent excitation of H-like heavy ions penetrating through a crystals.
Prosser (1998)	Energy spectrum of H atom in photon field.
Santos et al. (1998b)	Two-photon decay rates of $2s$-level in H-like ions. Z=1-100.
Shabaev (1998b)	TP between M1 hfs levels of H-like ions related to the bound-electron g-factor.
Shabaev et al. (1998a)	Recoil correction to H-like ground-state energy.
Shabaev et al. (1998b,1999)	Recoil correction to H-like energy levels.
Szmytkowski (1998a)	Continuum DC Sturmian functions.
van Lenthe et al. (1998)	Relation between Dirac and ZORA levels for M1 hfs, g-factors, of H-like systems.
Benvegnù (1999)	1D $-1/\|x\|$.
Holzscheiter and Charlton (1999)	Ultra-low energy antihydrogen. Review on experiments and possibilities.
Hua et al. (1999)	Exact, analytical solution of time-dependent Dirac equation.
Kónya and Papp (1999)	Coulomb Sturmian matrix elements of Coulomb Green's operators for KG and 2nd-order Dirac equations.
Moore (1999)	Magnetic shielding (NMR shift) for H-like Dirac atom. Closed-form expressions.
Vrejoiu et al. (1999)	Retardation corrections to angular distributions

Reference	Comments
	of free-bound transitions in H-like atoms.
Yamanaka and Ichimura (1999)	Nuclear polarizability contributions to $1s$ energies of H-like ^{208}Pb and ^{238}U. Transverse polarization is even more important than longitudinal one.
Yerokhin and Shabaev (1999)	First-order SE in H-like systems. $\|\kappa\| \leq 5$, $n \leq 5$. Uses DC Green function.

Table 2.4: The Dirac equation: Solutions for various non-Coulomb fields.

Reference	Comments
Gorshkov (1962)	Scattering of Dirac particle from Coulomb field with finite-nucleus and screening corrections.
Acker et al. (1966)	Muon in a two-parameter Fermi nuclear potential.
Gorshkov et al. (1967)	Screening effects in K-shell photoionization.
Mikhailov and Polikanov (1968)	Central potential. PT by reducing the Dirac equation to a Riccati equation.
Cook (1971)	Relativistic harmonic oscillator with intrinsic spin structure.
Coudray and Coz (1971)	Construction of V for fixed energy. KG and Dirac. The inversion problem.
Coulter and Adler (1971)	The 1D square-well potential.
Skyrme (1971)	Kinks and the Dirac equation.
Cusson et al. (1985)	Time-dependent 3D Dirac equation in heavy-ion scattering.
Bär (1990)	The spectrum of the Dirac operator.
Arai (1993)	Dirac-Weyl operator with a strongly singular gauge potential.
Artimovich and Ritus (1993)	Deep well potential.
Atanasov and Bankova (1993)	Relativistic Schrödinger equation in a linear +Coulomb potential.
Bautista (1993)	Dirac particle with anomalous magnetic moment μ' in a homogeneous magnetic field. Uniformly accelerated Rindler coordinates.
S. J. Blundell (1993)	The Dirac comb and the Kronig-Penney model.
Bosanac (1993)	Wave packets of spin-$\frac{1}{2}$ particles in an EM field.
Burgess and Jensen (1993)	Fermions near 2D surfaces. (3+1)D versus (2+1)D.
Caliceti and Cherubini (1993)	Relativistically deformed harmonic oscillator.
Centelles et al. (1993)	Dirac oscillator, $V(r) = \frac{1}{2}Kr^2$.
J.-J. Chang (1993,1998)	Dirac quantum-defect theory.
Z. Chen and Goldman (1993)	H-like atom with a finite nucleus in magnetic field.
Clerk and McKellar (1993)	Disordered 1D δ-function array.
Coutinho and Perez (1993)	Aharonov-Bohm scattering of Dirac particles by magnetic flux.
Crawford (1993)	Dirac oscillator and local automorphism invariance.
Droz-Vincent (1993)	Relativistic two-body problem in time-dependent external potentials.
Fujimoto and Kawakami (1993)	SO effects on persistent currents in mesoscopic Hubbard rings, threaded by an Aharonov-Bohm flux. Interplay of SO and $e-e$ interaction crucial.
Gambhir and Ring (1993)	Solution of Dirac equation using GTO basis for nuclei. Recipe for avoiding spurious states.
Gitman and Saa (1993)	Dirac-Pauli particle with anomalous magnetic momentum in external EM field.
J. Gonzalez et al. (1993)	Electronic spectrum of fullerenes from the Dirac equation.

Reference	Comments
Grigoryan and Grigoryan (1993)	Canonical quantization of Dirac particle in external magnetic field.
Hachem (1993)	Zeeman effect for Dirac electron.
Hatsugai and Lee (1993)	Localization of Dirac fermions in a 2D lattice.
Hersbach (1993a)	Relativistic calculations in momentum space. 'From positronium to quarkonium'.
Hersbach (1993b)	Relativistic linear potential in momentum space.
L. M. Jones (1993)	Another Dirac oscillator.
S. H. Kim (1993)	Thomson scattering by a relativistic electron.
Koutroulos and Papadopoulos (1993)	Dirac equation for rectangular spherical well. Model for hypernucleus.
Ktitarev and Yegikian (1993)	Feynman path integral for Dirac system with analytic potential.
Le and Nguyen (1993)	H-like atom in Dirac monopole + Aharonov-Bohm field.
Maier et al. (1993)	Time-dependent 1D Dirac square well: Pair production.
Matrasulov et al. (1993)	Near-continuum states of relativistic electron in an electric dipole field.
Maung et al. (1993)	Two-body system with confining linear+Coulomb interactions.
McQuarrie and Vrscay (1993)	KG equation with Coulomb + perturbing vector or scalar λr^k potentials. Rayleigh-Schrödinger PT of arbitrary order.
Mohamed et al. (1993)	Dirac operator with periodic potential. Asymptotic band spectrum.
Moshinsky and Loyola (1993)	Barut equation for particle-antiparticle system with Dirac oscillator interaction.
Nogami and Toyama (1993)	Supersymmetry aspects of 1D Dirac equation with a Lorentz scalar potential.
Ovcharov and Fedosov (1993)	Correlated coherent states of electron in field of plane EM wave.
Papp (1993a)	Dirac-Coulomb and linear potentials using 'β functions'.
Piekarewicz (1993)	Levinson theorem for Dirac particles.
Poliatzky (1993ab,1994)	Levinson theorem for Dirac equation.
Rosenberg and Zhou (1993)	Dirac and KG particles in a multimode laser field: Generalized Volkov solutions.
Roy (1993ac)	Boundary conditions at a δ-function in a 1D Dirac equation.
Roy (1993b)	Tunneling through a double δ-function barrier.
Roy and Khan (1993a)	Relativistic effects on impurity states.
Roy and Khan (1993b)	Relativistic effects on tunneling through multi-barrier systems.
Roychoudhury and Panchanan (1993)	Modified $1/N$ expansion for the Dirac equation for a screened Coulomb potential.
Safonov (1993)	Crystal-field anisotropies handled via the metric tensor of the space-time, for Dirac electrons.
Sakamoto (1993)	$N-$body bound state solution of Dirac particles in (1+1)D.
Salamin (1993)	Dirac particle with anomalous magnetic moment in a plane EM field.
Schmidt (1993)	Nonvanishing instability intervals in periodic Dirac systems.
Semay and Ceuleneer (1993)	Two-body Dirac equation and Regge trajectories.
Semay et al. (1993)	Two-body Dirac equation with diagonal central potentials.
Shabaev (1993a)	Finite-nuclear-size corrections to energy levels of multicharged ions. Expressed in terms of nuclear $\langle r^n \rangle$; n=2,4. Z=1-100.

Reference	Comments
Shishkin and Villalba (1993)	Electrically neutral Dirac particles in external fields. Exact solutions. Neutron in magnetic field.
Suzuki and Nogami (1993)	Variable-phase approach to the Dirac bound states.
Tashkova and Donev (1993)	Relativistic electron tunneling through structured 1D barrier.
Toyama et al. (1993)	Construct a 1D transparent potential of Lorentz scalar type. An infinite family exists.
Vonsovskii and Svirskii (1993)	Klein paradox and zitterbewegung for electron in a field with constant scalar potential.
Vonsovskii et al. (1993)	Electron zitterbewegung in linear crystal with alternating parity.
Willis (1993)	"Classical description of the absence of bound states for strong Coulomb fields."
Yao and Chu (1993)	Pseudospectral methods for bound and resonance state problems with the Dirac equation. H-like atom as example.
Zarzo and Martínez (1993)	Quantum relativistic harmonic oscillator. Spectrum of zeros in its wave functions from WKB.
Arvieu and Rozmej (1994, 1995)	"Spin-orbit pendulum": transitions from pure to mixed spin states.
Bagrov et al. (1994ab)	Maslov's 'complex germ method for a Dirac particle at the $\hbar \to 0$ limit.
Barut and Duru (1994)	Path-integral quantization for confined two-body problem.
Benvegnù and Dąbrowski (1994)	Relativistic point interaction.
Bergerhoff and Soff (1994)	Scalar potentials in the Dirac equation.
Bortman and Ron (1994)	Hysteresis in an atomic system (trapped ion, driven by a laser).
Clarkson (1994)	Spheres, pseudospheres.
Clemence (1994a)	Periodic Dirac system.
Clemence (1994b)	Levinson theorem for perturbed Coulomb potential.
Friedberg et al. (1994)	A new way of removing fermion doubling for solutions of the Dirac equation on a lattice.
A. Gonzalez et al. (1994)	Particle-antiparticle system with a Dirac oscillator interaction.
Grypeos et al. (1994,1995)	Dirac equation for neutrons in nuclei or Λ-particles in hypernuclei solved. Spherical, rectangular scalar and vector wells.
Helffer and Parisse (1994)	Decay of eigenfunctions for Dirac and KG. Tunneling.
Hersbach (1994)	Relativistic meson spectroscopy in momentum space.
Idlis et al. (1994)	Application of supersymmetry and factorization in solution of the Dirac equation.
Mijatović et al. (1994)	Scattering and bound states of a relativistic, neutral spin-$\frac{1}{2}$ particle in a magnetic field. System of N magnetic barriers or magnetic δ functions.
Khasanov (1994)	Constructs scalar and vector potentials for the Dirac equation with discrete eigenvalues in the continuum part.
Kwato Njock et al. (1994)	Supersymmetry-based QDT of Dirac equation for central potentials.
Z.-F. Luo et al. (1994)	Energy-dependent potential and hyperfine mass splitting of quarkonium.
Mattes and Sorg (1994)	Relativistic Schrödinger equation and the Bohm-Aharonov effect. Scalar localization field + extended vector field.

Reference	Comments
Melić (1994)	Hydrogenic atom with spinless nucleus in magnetic field.
W. Moreau et al. (1994)	Relativistic 1D harmonic and anharmonic oscillator.
C. Müller (1994)	Finite-element solution of time-dependent Dirac equations.
Müller-Nehler and Soff (1994)	Electron excitations in superheavy quasimolecules.
Nag and Roychoudhury (1994)	Exact solutions of two body Dirac equations.
Nagel (1994)	Relativistic Hermite polynomial is a Gegenbauer polynomial. Eigenfunctions of the 1D harmonic oscillator.
Newton (1994)	Comment on Poliatzky (1993ab).
Qian and Su (1994)	SO interaction and Aharonov-Anandan phase in mesoscopic rings.
Rosenberg (1994a)	Infrared radiative corrections to potential scattering of a Dirac electron.
Rosenberg (1994b)	Minimum principle for potential scattering of Dirac electron.
Roy (1994)	Tunneling through a multiple δ-function barrier.
Roy et al. (1994)	Relativistic equation for a slowly varying potential.
D. K. Roy and Singh (1994)	Relativistic effects on the tunnel effect.
Scherer et al. (1994)	Low-energy Compton scattering by a Dirac proton with anomalous magnetic moment. FW used.
Shabaev (1994a)	M1 and E2 hfs of H-like ions. Finite-nucleus corrections.
Sørensen and Belkacem (1994)	DC wave functions in momentum space.
Teychenné et al. (1994)	Oscillatory relativistic motion in a power-law or sinusoidal potential well. Classical (non-quantum).
Villalba (1994a)	Exact solution of the 2D Dirac oscillator.
Villalba (1994b)	Dirac equation for central fields. Separation in standard or rotating coordinate systems.
Villalba (1994c)	KG H-atom in magnetic monopole and Aharonov-Bohm potentials.
Waxman (1994)	Fredholm determinant for Dirac operator. 1D, some $V(x)$. Periodic boundary conditions.
Young and Norrington (1994)	Solution of relativistic asymptotic equations in electron-ion scattering. Program.
Zakout and Sever (1994)	Relativistic, heavy $q\bar{q}$ bound states. Parametrized effective potentials.
Baltz (1995)	Coulomb potential from a particle in uniform ultrarelativistic motion.
Cooper et al. (1995)	Supersymmetry and the Dirac equation. Coulomb and Lorentz scalar potentials. Magnetic field.
Danilov (1995)	Periodic potential. Resolvent estimates and spectrum.
Delbourgo (1995)	Square root of the harmonic oscillator.
Dominguez-Adame and Rodriguez (1995)	A 1D screened Coulomb potential.
Grigoryan and Grigoryan (1995)	Quasiclassical FW transformation and canonical quantization of $D = 2n$-dimensional relativistic particles in external EM field.
Halasz and Verbaarschot (1995)	Kalkreuter's (1995) Dirac spectrum for $SU(2)$ gauge theory. Statistical analysis of eigenvalues.
Kalkreuter (1995); Kalkreuter and Simma (1996)	Spectrum of squared Dirac operator using multigrid or conjugate gradient algorithms. $SU(2)$ gauge fields.
Kholomaj (1995,1998)	Dirac electron in arbitrary periodic electrostatic field.

Reference	Comments
Le Yaouanc et al. (1995)	High-order expansion of eigenvalues of a relativistic Coulomb equation.
A. Martin and Stubbe (1995)	Dirac equation for spherically symmetrical vector potential. Bargmann- and Calogero-type bounds for number of eigenvalues. Dito for KG.
Momberger et al. (1995)	Numerical, momentum-space solution of time-dependent Dirac equation for Au^{79+} or U^{92+} impinging on U^{91+}.
Moshinsky et al. (1995)	Two-body system with Dirac oscillator interaction. Symmetry Lie algebra.
Nana Engo et al. (1995)	Relativistic semiclassical dipole matrix elements for $nlj \to n'l'j'$ transitions in non-hydrogenic ions.
Panchanan et al. (1995)	$V(r) = -\frac{1}{r} + kr + gr^2$, $V(r) = -(1+\beta)/r$ solved. Reviews analytical solutions.
Rosenberg (1995)	Electron scattering by heavy hydrogenic ion.
Sucher (1995)	Confinement in relativistic potential models.
Tezuka (1995)	Dirac equation with attractive monomial (ar^n) or polynomial vector potential cannot confine a particle. A scalar potential, larger than vector potential, is needed.
Villalba (1995)	Dirac H-atom in magnetic monopole and Aharonov-Bohm potentials. Exact solution.
Alberto et al. (1996)	Relativistic particle in a 1D box. Avoid Klein paradox by a Lorentz scalar potential.
Avetissian and Movsissian (1996)	Scattering of Dirac electrons in arbitrary static potentials. Short- and long-range.
Camarda (1996)	Eigenvalues for quaternion matrix with a band structure.
Falomir et al. (1996)	Determinants of Dirac operators with local boundary conditions. 2D disk under baglike conditions.
Funakubo et al. (1996)	Numerical approach to CP-violating Dirac equation.
D.-S. Guo et al. (1996)	Dirac electron in multimode quantized radiation field.
Hagen and Park (1996)	Relativistic, (2+1)D Aharonov-Bohm-Coulomb problem. $1/r$, scalar and vector.
Kegley et al. (1996)	Deformed spherical oscillator with strong SO. Schrödinger equation solved in a lattice. Cylindrical coordinates.
J.-H. Kim et al. (1996)	Construct a potential for a constant-period classical (non-quantum) oscillator.
Lévai and Del Sol Mesa (1996)	Transform the Dirac equation into a Schrödinger-like one for minimal and non-minimal couplings. Polynomial potentials.
Maksudov and Allakhverdiev (1996)	Spectral theory of non-self-adjoint Dirac operators.
T. A. Marian (1996)	Higher-order multipole expansions for Dirac and Pauli Hamiltonians. (Atomic electron in radiation field). Includes retardation up to 4th order.
Nenciu and Purice (1996)	1D periodic Dirac Hamiltonians: semiclassical and high-energy asymptotics for the gaps.
Nogami and Toyama (1996)	Coherent state of the Dirac oscillator.
Ogurisu (1996)	Neutral Dirac particle with anomalous magnetic moment in asymptotically constant magnetic field.
Protopapas et al. (1996,1997)	Atomic physics with super-high intensity lasers. Important mass-shift effects.

Reference	Comments
Roy (1996)	'Fibonacci lattice' of rectangular potential wells.
Savchenko (1996)	Dirac particle with anomalous magnetic moment in a circularly polarized wave.
Szmytkowski and Hinze (1996)	NR and R R-matrix expansions at the reaction volume boundary.
Tkachuk and Vakarchuk (1996)	The N=4 supersymmetry of electron in magnetic field.
Valiev and Pazdzerskij (1996)	Dirac equation for a singular point potential.
Znojil (1996)	Harmonic oscillations in quasirelativistic regime. $V(r) = \sqrt{A + Br^2}$.
Alonso and De Vincenzo (1997);	Dirac particle in a 1D box.
Alonso et al. (1997)	1D or spherical box. Boundary conditions discussed.
Bose (1997)	Relativistic Schrödinger equation, $V(r) = -\alpha/r + \beta/r^{1/2}$.
Cotaescu and Draganescu (1997)	Operator algebra of the relativistic oscillator.
Falsaperla et al. (1997)	Two methods for solving the Dirac equation without variational collapse (Lehmann-Maehly and Kato methods). H atom in magnetic field.
Karat and Shulz (1997)	Self-adjoint extensions of the Pauli equation in presence of magnetic monopole.
Khelashvili and Kiknadze (1997)	Bound states in the continuum for quasipotentials, arising from QED.
Kylstra et al. (1997)	1D Dirac model atom in an intense laser field. Time-dependent problem solved in momentum space using B-splines.
R. T. Lewis et al. (1997)	Essential spectrum of relativistic multi-particle operators.
Lieb et al. (1997ab)	Stability of matter in classical EM fields. (Dirac electrons).
D.-H. Lin (1997)	Relativistic fixed-energy amplitudes of step and square well potentials.
Lobanov (1997)	Electron polarization in a pulsed EM field.
Lun and Buckman (1997);	Extract SO interactions from scattering phase
Lun et al. (1998)	shifts via inversion. Obtain effective $V_{\mathrm{SO}}(r)$.
Olsen and Kunashenko (1997)	Channeling of relativistic electrons in crystals. Electron-positron production. Dirac equation in cylindrical coordinates.
Qian et al. (1997)	Persistent currents from competition between Zeeman coupling and SO interaction.
Rathe et al. (1997)	Intense laser-atom dynamics with 2D Dirac equation.
Rozmej et al. (1997)	'Collapse and revival' in wave-packet dynamics due to SO interaction.
Rutkowski and Kozlowski (1997)	Relativistic H atom in static, uniform **B**. DPT.
Skarzhinsky and Audretsch (1997)	Scattering of scalar and Dirac particles by a magnetic tube of finite radius.
Stahlhofen (1997)	Algebraic solutions of DC problems. Symmetries. Relations with Dirac oscillators.
Torres del Castillo and Cortés-Cuautli (1997)	Dirac equation in the field of a magnetic monopole.
Toyama et al. (1997)	The Dirac harmonic oscillator under a FW transformation.
Villalba (1997)	Exact solution of Dirac equation for pseudoscalar potentials: 1D $1/x$, cylindrical $1/\rho$, spherical $1/r$. No bound states.
Vonsovskii and Svirskii (1997)	Zitterbewegung and uncertainties of velocity and acceleration in Dirac theory.

Reference	Comments
Wachter et al. (1997)	Relativistic corrections to the central $q\overline{q}$ potential in meson theory.
Alberto et al. (1998)	Infinite spherical well. Uses Lorentz scalar potential. Discuss LS coupling.
Arbatsky and Braun (1998)	Quadratic Zeeman effect for highly excited H.
Asaga et al. (1998)	g-factor of a tightly bound electron.
Atakishiyev et al.(1998)	Meixner oscillators. Have equidistant levels.
Barakat et al. (1998)	Perturbed Coulomb potentials in the KG equation.
Berbenni-Bitsch et al. (1998)	Microscopic universality in spectrum of lattice Dirac operator.
Bruce and Roa (1998)	Dirac particle in a vectorlike Coulomb potential.
Dattoli et al. (1998)	'Relativistic Hermite polynomials'.
Dragić et al. (1998)	H atom with added magnetic SO and spin-spin interactions. No deep-lying extra levels found.
Ermolaev (1998)	3D potentials for atoms in superintense laser fields.
X.-C. Gao et al. (1998)	KG particle in time-dependent, homogeneous **E**.
Huber and Leeb (1998); Huber (1995)	SO potentials from inversion of radial Dirac equations.
Lichnerowicz (1998)	First eigenvalue of Dirac operator for Kähler manifold of even complex dimension.
Q.-G. Lin (1998)	Levinson theorem for a 2D Dirac particle in a central field.
Mallampalli and Sapirstein (1998c)	Solves $H = \sqrt{\mathbf{p}^2 + m^2} - m - \frac{Z\alpha}{r}$ in momentum space using B-splines. No singularity problems in **p**-space
Milhorat (1998)	Spectrum of the Dirac equation on Gr_2 (C^{m+2}).
Mudry et al. (1998)	2D Dirac particle in strong imaginary vector potential + random impurity potential.
C. Müller et al. (1998)	Finite-element solution of 1D time-dependent Dirac equations. A solution for 'fermion doubling'.
Nedjadi et al. (1998)	Extended relativistic oscillator for $S = 1$ particles.
Nikitin (1998)	New classes of external fields having an exact FW transformation.
Nogami and Toyama (1998)	Reflectionless potentials for 1D Dirac equation. Pseudoscalar potentials.
Pal'chikov (1998)	En and Mn TP of arbitrary n for H-like atoms. Z=1-92.
Schön and Köppel (1998)	Geometric phases and quantum dynamics in SO-coupled systems. Molecules with vibronic interactions.
Segev and Wells (1998)	Time-dependent Dirac equation solved at ultrarelativistic limit for pair production in heavy-ion collisions. Light-front variables.
Sugawara-Tanabe and Arima (1998);Sugawara-Tanabe et al. (1999)	Hidden pseudospin symmetry in the Dirac equation. Spherical or axially deformed potentials.
Szmytkowski (1998b)	Variational R-matrix methods for the Dirac equation.
Taïeb et al. (1998)	Signature of relativistic effects in atom-laser interactions at ultrahigh intensities. 1D 'soft-core Coulomb' model: $V(x) = -q/\sqrt{2 + v^2}$. KG.
Villalba and Pino (1998)	2D hydrogen atom in magnetic field. KG and Pauli.
Wen et al. (1998)	High harmonics of H atom in ultrastrong laser field. MC simulation.
Yu and Takahashi (1998)	Dirac electron in two-frequency circularly polarized EM wave. Radiation and pair production.

Reference	Comments
Benvegnù (1999)	1D -1/|x|.
Bohun and Copperstock (1999)	Dirac-Maxwell solitons. Potential of uniformly charged sphere.
Brau (1999)	1D spinless Salpeter eq. for Coulomb + hard-core potential. Results wrong.
Braun et al. (1999)	Numerical solution of time-dependent Dirac equation. Split-operator method on a (3+1)D grid. Discuss the Klein paradox and the *Zitterbewegung*.
J. Chen et al. (1999)	High-order harmonics for H-like atom in ultrastrong laser field.
Darewych (1999)	Integral identities and bounds for scattering solutions.
Hall (1999)	Spectral comparison theorem for Dirac equation with $V(r)$.
Y. S. Huang et al. (1999)	Relativistic H-atom in spherical cavity. Applications to spherical quantum dots.
Kapshai and Alferova (1999)	1D scattering problem from superposition of δ-potentials.
D.-H. Lin (1999)	Path integral for the 3D Aharonov-Bohm-Coulomb system.
Q.-G. Lin (1999)	Levinson theorem for a 1D Dirac particle in a symmetrical field.
Matrasulov et al. (1999)	Dirac electron in the field of two opposite charges. $Z < 137$ and $Z > 137$ considered.
Mustafa and Odeh (1999)	KG for harmonic oscillator. Cp. Znojil (1996).
Narayan Vaidya and Barbosa da Silva Filho (1999)	Green function for charged spin-$\frac{1}{2}$ particle with anomalous magnetic moment in a plane wave EM field.
Nitta et al. (1999)	Motion of wave packet in Klein paradox.
Ouyang et al. (1999)	Dirac particles in twisted tubes.
Panek et al. (1999)	Electron scattering in powerful laser field. Angular and polarization effects. Electron handled as laser-dressed KG particle.
Rozmej and Arvieu (1999)	The Dirac oscillator. Permits exact FW.
Şimşek (1999)	Negative-energy levels for a ND Dirac equation. Spherically symmetrical, purely imaginary, linear potential.
Soliman and Abelraheem (1999)	Modification of band structure in intense laser fields. 1D model. New gaps introduced.
Toyama and Nogami (1999)	Search a 1D Dirac harmonic oscillator potential. (Only bound states, equally spaced.) Combination of scalar ($\beta S(x)$) and pseudoscalar ($\alpha\beta f(x)$) terms works.
Wessels et al. (1999)	Discretizing the 1D Dirac equation. Use time symmetry to conserve probability density.

Table 2.5: Relativistic virial theorems.

Reference	Comments
Rutkowski et al. (1993)	Relativistic virial theorem for diatomic molecules. H_2^+. Large-R and small-R limits.
Semay (1993)	Virial theorem for two-body Dirac equation.
Moiseiwitsch (1997)	Virial theorem for electron capture from H-like atom.
Cohen and Leung (1998)	Relativistic corrections to atomic sum rules using the FW approximation.
Cohen and Leung (1999)	Comment on Romero and Aucar (1998).

Chapter 3

Quantum Electrodynamical Effects

Table 3.1: QED and other higher-order effects: Methods.

Reference	Comments
Håkansson (1950)	Bethe logarithm for helium-like atoms.
Baranger et al. (1953)	Relativistic correction to Lamb shift. Hydrogen $2s$, 7.13 MHz.
Sommerfield (1958)	Electron g-factor to 4th order.
Todorov (1971)	Quasipotential equation in relativistic eikonal approximation.
Sapirstein and Yennie (1990)	Theory of hydrogenic bound states. Review.
Compagno and Salamone (1991)	Radiative corrections to charge density of an electron in an oscillator potential.
Shabad (1991)	VP and an electron gas in external field.
Crater et al. (1992); Crater and Van Alstine (1994)	Two-body interactions for spinning particles.
Milonni and Shih (1992b)	Casimir forces. Review.
K. T. Cheng et al. (1993)	Lamb shifts for non-Coulomb potentials. Finite nuclear size, core-Hartree potential.
Compagno et al. (1993)	Radiative corrections to charge density of H-like atoms. Main effect eigenvalue-induced exponential at large r. Related to Welton potential.
Devoto et al. (1993)	High-Z Lamb shifts in stripped atoms can be obtained from H-like values for a given electron density.
Frochaux (1993abc)	Relativistic corrections to Schrödinger equation from quantum field theory.
Hostler (1993,1994)	SE for an electron in an external potential. Commutator expansion. Reduced Green function.
Ionescu et al. (1993)	Collective excitations of the QED vacuum.
Ito and Gross (1993)	Compton scattering from relativistic composite systems.
Khriplovich et al. (1993)	Logarithmic corrections in the two-body QED problem.
Labzowsky (1993)	Adiabatic S-matrix approach in QED of large-Z He-like ions.
Labzowsky et al. (1993a)	Review on higher-order QED corrections for high-Z ions.
Labzowsky et al. (1993b)	Treatise on relativistic and QED effects in atoms.
Lindgren et al. (1993b)	2nd-order QED corrections for few-electron atoms. Reducible Breit-Coulomb correction and mixed SE-VP correction.
Lindgren et al. (1993c)	Bound-state SE using partial-wave renormalization.
Mohr (1993,1994)	QED in few-electron systems.
Pachucki (1993a)	QED corrections to charge density in H-like atoms.
Pachucki (1993b)	Two-loop corrections to Lamb shift of s-states.
Pachucki (1993c)	Higher-order binding corrections to Lamb shift.
Pachucki et al. (1993)	Nuclear-structure correction to the Lamb shift are -60 Hz and -19 kHz for H and D $1s$, respectively.
Persson (1993)	QED effects in highly charged ions. Thesis.
Persson et al. (1993a, 1998)	New approach to SE calculations. Convergent sums for each partial wave. H-like ions, Li-like U.
Persson et al. (1993b)	Accurate calculation of higher-order VP terms (beyond Uehling potential). Can be used with arbitrary atomic potential.
Quiney and Grant (1993,1994)	Partial-wave mass-renormalization in atomic QED calculations.
Rosenberg (1993)	Derives effective Hamiltonian for a two-electron atom. Extremum principles.

Reference	Comments
Sapirstein (1993)	Theory of many-electron atoms. Review on QED and many-body aspects.
Schneider et al. (1993a)	Källén-Sabry energy shift for H-like atoms with finite nuclei. (The VP shift of order $\alpha^2(Z\alpha)$). Z=1-100.
Seke (1993)	Gauge independence of NR Lamb shift including retardation effects.
Shabaev (1993b)	A Schrödinger-like equation derived from QED for the relativistic few-electron atom.
Soff (1993)	Radiative corrections in strong Coulomb fields. Emphasizes higher-order VP, nuclear-size effects on SE.
Sommerer (1993)	Relativistic two-body wave equations.
Yakhontov and Grant (1993)	Parameter-free renormalization in self-mass correction.
Barut and Saradzhev (1994)	Two-body system in (1+1)D QED.
Cavicchi and Vairo (1994)	New method for Lamb-shift calculation.
Hnizdo (1994)	VP potentials for extended nuclear charges.
Khriplovich et al. (1994)	Infrared divergence, Thomson scattering and the Lamb shift.
Kijowski (1994)	On electrodynamical self-interaction.
Labelle et al. (1994)	$O(m\alpha^8)$ contributions to decay of orthopositronium.
Labzowsky et al. (1994)	Non-resonant corrections (deviation of line profiles from Lorentz form) in Lamb-shift measurements for high-Z H-like ions.
Mil'shtein and Khriplovich (1994)	Large relativistic corrections to positronium decay.
Padden (1994)	Coulomb correction to VP tensor in superstrong $\mathbf{B}$.
Rosenberg (1994a)	Infrared radiative corrections to potential scattering of a Dirac electron.
Schweber (1994)	History of QED.
Seke (1994)	Spontaneous decay of excited atomic states in NR QED.
Shabaev (1994b)	QED theory of electron recombination with highly charged ions.
Tang and Finkelstein (1994)	Relativistically covariant symmetry in QED.
Aucar et al. (1995b)	Bethe sum rule for the no-pair Hamiltonian.
Acikgoz et al. (1995)	Calculation of VP using self-field QED without infinities.
Hartemann and Luhmann (1995)	Radiation damping force on accelerated charged particle.
Kinoshita (1995)	New value for α^3 electron anomalous magnetic moment.
Koures and Harris (1995)	Gaussian-basis QED.
Labzowsky and Tokman (1995)	Reference state two-photon corrections for high-Z few-electron ions. Applications on Li-like ones.
Lindgren et al. (1995a)	Full QED calculation of two-photon exchange in He-like systems.
Mitrushenkov et al. (1995)	2nd-order loop-after-loop SE correction for few-electron multicharged ions.
Pachucki (1995)	Radiative recoil correction to Lamb shift.
Pachucki and Karshenboim (1995)	Nuclear-spin-dependent recoil correction to Lamb shift.
Rivelles (1995)	Comments on nonlocal and covariant symmetry in QED.
Rocchi and Sacchetti (1995)	Radiative corrections to Compton cross section.

Reference	Comments
Schäfer and Reinhardt (1995)	VP as test of C and CPT invariance. Muonic $4f_{7/2}$ and $5g_{9/2}$ levels in ^{209}Pb.
Eides (1996)	Weak-interaction contributions to hfs and the Lamb shift.
Jentschura and Pachucki (1996)	Higher-order Lamb shifts of $2P$ states.
Khriplovich et al. (1996)	Nature of the Darwin term and $(Z\alpha)^4 m^3/M^2$ contribution to the Lamb shift for arbitrary spin of the nucleus.
Kinoshita (1996)	The fine structure constant, α.
Labzowsky (1996)	Treatise on QED of atoms.
Labzowsky and Mitrushenkov (1996)	2nd-order SE for tightly bound atomic electron.
Labzowsky et al. (1996)	Vacuum polarization-nuclear polarization corrections to the Lamb shift.
Mallampalli and Sapirstein (1996)	4th-order VP contribution to Lamb shift. Z=5-100.
Mohr (1996)	Tests of fundamental physics.
Pachucki (1996a)	Lamb shift in muonic hydrogen.
Pachucki et al. (1996)	Theory of energy levels of H and D.
Pak et al. (1996)	D-line of Na-like ions. Includes a phenomenological Lamb-shift model.
Persson et al. (1996a)	Second-order SE-VP contributions to Lamb shift. H-like and Li-like systems, Z=70...92.
Persson et al. (1996b)	Two-electron Lamb shifts for He-like ions.
Sapirstein (1996a)	Quantum electrodynamics.
Seke (1996)	Complete Lamb shift to order α^5 in NR QED.
Shelyuto (1996)	Suggests a new gauge for the photon propagator. One-loop radiative corrections.
Beier et al. (1997a)	Review on Lamb shifts of H-like ions.
Beier et al. (1997b)	Two-loop VP contribution for H-like ions.
Beier et al. (1997c,1998)	Influence of nuclear size on QED corrections of H-like ions.
Blundell et al. (1997a)	Effects of non-Coulomb fields on radiative corrections. Electron screening, Zeeman field, M1 hyperfine fields as example.
Gonzalo and Santos (1997)	Radiative corrections to Zeeman effect of 2 ^3P states of He.
Hylton and Snyderman (1997)	Analytic basis set for high-Z atomic QED. He-like ions. Sturmian DC functions.
Jaekel and Reynaud (1997)	Movement and fluctuations of the vacuum.
Jallouli and Sazdjian (1997a)	Two-body potentials for two spin-0 or spin-$\frac{1}{2}$ particles from summation of Feynman diagrams.
Jallouli and Sazdjian (1997b)	Incorporation of anomalous magnetic moments.
Jentschura et al. (1997a)	Bound $\mu^+\mu^-$ system.
Jentschura et al. (1997b)	Lamb shift of $3P$ and $4P$ states and the determination of α.
B. D. Jones and Perry (1997)	Lamb shift in a light-front Hamiltonian approach.
Karshenboim (1997c)	Radiative corrections to light muonic atom decay.
Khelashvili and Kiknadze (1997)	Bound states in the continuum for quasipotentials, arising from QED.
Labzowsky and Goidenko (1997)	Multiple commutator expansion for the Lamb shift in a strong Coulomb field.

Reference	Comments
Labzowsky et al. (1997b)	Non-resonant QED corrections to radiative electron capture of highly charged ions.
Mohr (1997)	QED corrections in heavy atoms.
Persson et al. (1997b)	Theoretical survey of QED tests in highly charged ions.
Quiney et al. (1997)	Relativistic calculation of EM properties of molecules.
Stöcker et al. (1997)	Structure of vacuum and elementary matter. Conference proceedings.
Tulub et al. (1997)	Simulate the QED effects in many-electron atoms by a renormalized nucleus (right radius, changed charge inside).
Yerokhin et al. (1997a)	Two-electron SE contribution to the ground-state energy of He-like ions.
Au and Chu (1998)	H-like atoms with finite mass: two-photon processes lead to effective scalar photon interaction.
Dmitriev and Fedorova (1998)	New adiabatic QED method for bound states. Applied on two-photon exchange diagrams.
Dmitriev et al. (1998)	New, direct renormalization of bound electron self-energy.
Greiner (1998)	Correlations in the vacuum.
Jallouli and Sazdjian (1998)	Relativistic effects in pionium ($\pi^+\pi^-$) lifetime. Corrections of order $O(\alpha)$.
Karshenboim et al. (1998b)	One-loop VP correction to energy and wave function at origin in exotic atoms.
Khriplovich et al. (1998)	$O(\alpha^7(\ln\alpha)mc^2)$ corrections to FS splittings and $O(\alpha^6(\ln\alpha)mc^2)$ corrections to He energy levels. (Comment on T. Zhang (1996)).
Khriplovich and Sen'kov (1998)	Nucleon polarizability contribution to H-atom Lamb shift and H-D isotope shift.
Labzowsky et al. (1998a)	SE with partial-wave renormalization using B-splines. Results for H-like ns ions, Z=10-100, n=1-8.
Labzowsky et al. (1998bc)	2nd-order SE counterterms in bound-state QED.
Labzowsky and Tokman (1998)	Reference state two-photon Coulomb-Breit corrections for high-Z few-electron ions. Applications on Li-like ones.
Lindgren et al. (1998)	Analysis of SE for tightly bound electrons.
Low (1998)	Run-away electrons in relativistic spin-$\frac{1}{2}$ QED.
Mallampalli and Sapirstein (1998a)	4th-order SE contribution to Lamb shift.
Mallampalli and Sapirstein (1998b)	Perturbed-orbital two-loop Lamb shift. Z=0.5-5.
Mallampalli and Sapirstein (1998c)	Bethe logarithm for hydrogen using B-spline basis.
Mickelsson (1998)	VP and the geometric phase: Gauge invariance. Quantized fermions in external vector potentials.
Moussa and Baseia (1998)	Nonlocality of single photon in cavity QED.
Pachucki (1998a)	Energy of He $n\,^3S_1$ states in order $m\alpha^6$. Effective Hamiltonian approach. Regularized Coulomb, $V(R) = -\frac{Z\alpha}{r}(1 - \mathrm{e}^{-\lambda m\alpha r})$.
Pachucki (1998b)	Singlet S states of He to order $m\alpha^6$.
Pachucki (1998c)	Simple derivation of He Lamb shift.
Pachucki and Karshenboim (1998)	Positronium to order $m\alpha^6$.

Reference	Comments
Passante (1998)	Level shifts of accelerated H atom. Contribution from vacuum fluctuations affected.
Persson et al. (1998)	Renormalization corrections to partial-wave procedure.
Plunien et al. (1998)	Exact two-loop VP correction to Lamb shift in H-like ions.
Pyykkö et al. (1998)	Estimated valence-electron Lamb shifts for Li-E119, Cu-E111. About -1% of kinetic Dirac shifts for large Z.
Sapirstein (1998)	Theory of many-electron atoms. Review on QED and many-body aspects.
Schaden et al. (1998)	Unified treatment of some Casimir energies and Lamb shifts. Lamb shift of an atom in a dielectric medium, like a dilute gas.
Seke (1998)	Spontaneous decay of excited atomic states in R/NR QED.
Shabaev (1998a)	QED theory of nuclear recoil in atoms to all orders in αZ.
Soff et al. (1998)	QED in strong fields. Review.
Sucher (1998)	What is the force between the electrons? Searches an effective electron-electron potential.
Sunnergren (1998)	Complete one-loop QED calculations for few-electron ions. Applications on energies, g-factors and hfs. Thesis.
Yerokhin et al. (1998)	Two-electron SE corrections to ground-state energy of Li-like ions, $Z = 20 - 100$.
Bach et al. (1999)	Stability of the relativistic electron-positron field.
Bednyakov et al. (1999)	Electroweak radiative corrections.
Beier et al. (1999)	QED effects on radiative electron capture.
Coutinho et al. (1999)	Two definitions for electric polarizability, with or without the vacuum background.
Hughes and Kinoshita (1999)	Anomalous g values of the electron and muon. A review.
Ionescu and Belkacem (1999)	Relativistic collisions of highly-charged ions. Time evolution of QED vacuum solved numerically.
Ionescu et al. (1999)	Inner-shell photoionization at relativistic energies. Vacuum-assisted processes most probable at high E. 'Vacuum spark'.
Jentschura et al. (1999)	Nonperturbative numerical evaluation of 1-photon SE for H-like ions with low Z of 1-5.
Labelle and Zebarjad (1999)	Derivation of Lamb shift using effective field theory.
Labzowsky et al. (1999a)	QED corrections to ns electron g factors of neutral K-Fr, Ba^+.
Milonni et al. (1999)	Lamb shift of an atom in a dielectric medium.
Nefiodov et al. (1999a)	New approach to electron SE. Based on multiple commutator expansion and partial-wave renormalization.
Nefiodov et al. (1999b)	QED effects of radiative interference in recombination of electrons with heavy multicharged ions. Dielectronic recombination of He-like U.
Pachucki (1999a)	QED effects on He FS.
Pachucki (1999b)	Proton structure effects in muonic hydrogen.
Pachucki and Karshenboim (1999)	Higher-order recoil corrections to energy levels of two-body systems.
Panat and Paranjape (1999)	Dipolar and quadrupolar contributions to SE of H-like atom between two metallic slabs.
Ritchie and Weatherford (1999)	Quantum classical correspondence in NR QED. Lamb shift of a harmonically bound electron.
Sapirstein et al. (1999)	Potential-independence in relativistic MBPT achieved

Reference	Comments
	if negative-energy states are included. He-like ions. 'No-pair' not enough.
Vrejoiu et al. (1999)	Retardation corrections to angular distributions of free-bound transitions in H-like atoms.
Webb et al. (1999)	Search for time variation of the fine-structure constant α.
Yerokhin et al. (1999a)	Two-electron SE correction to $2p_{1/2} - 2s$ transition energy in Li-like ions, $Z = 18 - 100$.
Yerokhin et al. (1999b)	Screened SE and VP in high-Z Li-like ions.
Yerokhin and Shabaev (1999)	First-order SE in H-like systems. $\|\kappa\| \leq 5$, $n \leq 5$, Z=74,83,90,92.

Table 3.2: QED: Hyperfine interactions.

Reference	Comments
Bodwin et al. (1985)	Reviews recoil effects in QED of hfs.
Bodwin and Yennie (1988)	Recoil corrections to hydrogen hfs.
G. Li et al. (1993)	One-logarithmic recoil in muonium hfs.
Kinoshita and Nio (1994); Nio and Kinoshita (1997)	Muonium hfs.
Schneider et al. (1994a)	VP contribution to M1 hfs of H-like atoms.
T. Zhang and Xiao (1994)	Positronium hfs, α^6 corrections.
Eides and Shelyuto (1995)	M1 hfs contributions of order $\alpha^2(Z\alpha)^5$.
Schneider (1995)	M1 hfs of one-electron atoms. Thesis.
Shabaeva and Shabaev (1995)	Interelectronic contribution to hfs of Li-like ions. $1/Z$ expansion, including QED effects. Z=5-100.
Labzowsky et al. (1995)	Introduce the 'dynamic proton model' for hfs of H-like ^{209}Bi. Interaction between valence electron and valence proton at QED level.
Karshenboim (1996b)	Leading logarithmic corrections to muonium hfs.
Pachucki (1996b)	$\alpha(Z\alpha)^2 E_F$ correction to M1 hfs in H-like atoms.
Persson et al. (1996c)	SE correction to hfs of H-like atoms.
Yan et al. (1996)	FC term of M1 hfs in Li $2s, 2p, 3s$, Be^+ $2s$. Includes QED.
Blundell and Cheng (1997b)	Muonium hfs splitting.
Karshenboim (1997a)	Nuclear-structure-dependent radiative corrections to hydrogen hfs.
Labzowsky et al. (1997ac)	M1,E2,M3 hfs of the $2p_{3/2}$ state of H-, Li-, B- and N-like $^{209}_{83}$Bi. Interaction between valence electron and valence proton treated at QED level.
Pachucki (1997)	Positronium hyperfine structure.
Persson et al. (1997a)	Radiative corrections to electron g-factor in H-like ions.
Shabaev et al. (1997b)	Ground-state M1 hfs splitting of H-like ions. Z=49-83.
Tulub et al. (1997)	Simulate the QED effects in many-electron atoms by a renormalized nucleus (right radius, changed charge inside). Application on M1 hfs of H-like Bi.
Yerokhin et al. (1997b)	SE correction to $1s$ and $2s$ hfs splitting in H-like ions.
Beiersdorfer (1998b)	M1 hfs in Li-like U.
Karshenboim et al. (1998ab)	Analytic Uehling correction to hfs of muonic atoms.
Shabaev et al. (1998c)	QED and nuclear effects in highly charged ions.
Shabaev et al. (1998e)	Ground-state M1 hfs splitting and lifetime for Li-like

Reference	Comments
	ions, Z=49-83. Includes QED.
Sunnergren et al. (1998)	Radiative corrections to hfs of H-like systems.
Czarnecki et al. (1999a)	Positronium hyperfine splitting. Analytical $O(m\alpha^6)$.
Czarnecki et al. (1999b)	α^2 Corrections to parapositronium decay.
Faustov et al. (1999)	Hadronic VP and muonium M1 hfs.
Shabaev (1999)	Hfs of highly charged (H- and Li-like) ions. By combining them, nuclear factors can be eliminated. TP. QED included.

Table 3.3: QED: Energy levels.

Reference	Comments
Acker et al. (1966)	VP for muons in a Fermi nuclear potential.
Fricke (1969)	VP in muonic atoms. Quadrupole part of VP, muonic or pionic pairs included.
Geersten (1969)	Lamb shift and vibrational spectra of H_2^+, HD^+.
Jeziorski and Kołos (1969)	H_2^+ Lamb shift and the IP of H_2.
Blomqvist (1972)	VP in exotic atoms. Muonic Pb.
Feldman and Fulton (1988)	Lamb shifts for many-electron atoms.
Klarsfeld (1977)	Analytical expressions for VP in muonic atoms.
Kim et al. (1991)	Lamb-shifts for resonance transitions of Li-, Na- and
[=Ref. 4829 in RTAM II]	Cu-like ions.
Bukowski and Jeziorski (1993)	Lamb shift for muonic H_2^+ (ppμ etc.).
Beiersdorfer et al. (1993,1998b)	The $2s_{1/2} - 2p_{3/2}$ Lamb shift in Li-like to Ne-like U.
Berry et al. (1993)	QED and $1s2s$ - $1s2p$ triplet state energies of He-like systems, Z=2-92.
Berseth and Darewych (1993)	QED corrections to Ps^-.
Blundell (1993ab);	QED effects in Li-like, Na-like and Cu-like ions.
Blundell (1994)	Screening effects included.
Blundell (1993c)	Two-photon graphs for He-like ions.
Drake et al. (1993)	Energy corrections of order $mc^2\alpha^6 \ln\alpha$ for He.
Fell (1993)	Single-transverse-photon contributions of order $\alpha^6 \ln\alpha$ to energy levels of positronium.
Babb and Spruch (1994)	Retardation (Casimir) potential for Rydberg H_2 from QED.
Eides et al. (1994)	Light-by-light-scattering $\alpha^2(Z\alpha)^5 m$ contribution to H-atom Lamb shift.
Haftel and Mandelzweig (1994a)	Relativistic, finite-size and QED corrections for the $2\ ^1S$ state of He.
Shabaev and Fokeeva (1994)	Reducible part of two-photon diagrams in the QED of multicharged ions.
Artemyev et al. (1995ab)	Nuclear recoil corrections for H-like and Li-like systems to all orders of αZ.
Adkins and Shiferaw (1995);	Positronium hyperfine levels
Eides and Grotch (1995ab)	α^6 corrections to S levels.
Eides and Shelyuto (1995)	Lamb-shift contributions of order $\alpha^2(Z\alpha)^5$.
Johnson et al. (1995)	$2s_{1/2} - 2p_{3/2}$ transitions in Li-like to Ne-like U. Includes one-loop QED corrections.
Kukla et al. (1995)	He-like Ar^{16+}, $1s2s\ ^3S$ - $1s2p\ ^3P$. Uncalculated QED terms estimated as $0.15(Z\alpha)^4$ a.u.
Eides (1996)	Weak-interaction contributions to hfs and the Lamb shift.
Erokhin and Shabaev (1996)	Screened SE diagrams to ground-state Lamb shift of

Reference	Comments
	two-electron atoms.
Nefiodov et al. (1996)	Nuclear polarization effects on spectra of multicharged ions. H-like ^{208}Pb, ^{238}U. Effects small.
Pak et al. (1996)	D-line of Na-like ions. Includes a phenomenological Lamb-shift model.
M. S. Safronova et al. (1996a)	$n = 2$ levels of Be-like systems, Z=4-100. Includes Lamb shift.
M. S. Safronova et al. (1996b)	$n = 2$ levels of B-like systems, Z=5-100. Includes Lamb shift.
T. Zhang (1996ab, 1997); T. Zhang and Drake (1994ab,1996)	QED corrections to FS of He.
Adkins et al. (1997); Adkins and Sapirstein (1998)	Positronium hyperfine interval.
Artemyev et al. (1997)	VP screening corrections for He-like ground states.
Beier et al. (1997a)	Review on Lamb shifts of H-like ions.
Beier et al. (1997c, 1998)	Influence of nuclear size on QED corrections of H-like ions.
Bhatia and Drachman (1997)	Rydberg states of Li.
Eides and Grotch (1997a)	Recoil corrections of order $(Z\alpha)^6(m/M)m$ to H-like s levels.
Eides and Grotch (1997b)	Radiative correction to nuclear-size effects and isotope shifts.
Eides et al. (1997)	Lamb-shift contribution of order $\alpha^2(Z\alpha)^5 m$
Elander and Yarevsky (1997)	QED corrections for antiprotonic helium.
Friar and Payne (1997a)	Higher-order nuclear-polarizability corrections for hydrogen (H or D).
Friar and Payne (1997b)	Higher-order nuclear-size corrections for hydrogen.
V. G. Ivanov and Karshenbojm (1997a)	Radiative corrections to level widths of light mesonic atoms.
V. G. Ivanov and Karshenbojm (1997b)	VP contribution of order $\alpha(Z\alpha)^6 mc^2$ to H-like levels
Karshenboim (1997a)	Two-loop logarithmic corrections in hydrogen Lamb shift.
Karshenboim (1997b)	Lamb shift of excited s levels of H and D.
King (1997,1999)	High-precision calculations on the Li atom. Review.
Korobov and Bakalov (1997)	Metastable states of antiprotonic He.
Martynenko and Faustov (1997)	FS of positronium.
Pal'chikov et al. (1997)	Assesses accuracy of Lamb-shift measurements in H.
M. S. Safronova et al. (1997ab)	$n = 3$ levels of Be-like systems, Z=4-30,54. Includes Lamb shift.
Yan and Drake (1997)	FS of Li $2p$ state. Includes QED.
Yan and Drake (1998)	Relativistic and QED energies in Li $2s$, $2p$ states and in Li^+.
Beiersdorfer et al. (1998)	The $2p_{1/2} - 2p_{3/2}$ transition of Be-like to F-like U.
Bhatia and Drachman (1998a)	Lamb shift in two-electron systems. He-like ground-states, $Z \leq 10$.
Indelicato et al. (1998)	K-, L-, and M-shell IP for elements with Z=10-100. The $1s$ Lamb shift of heavy elements.
Indelicato and Mohr (1998a)	Coordinate-space approach to bound-electron SE. Coulomb-field calculation.
Indelicato and Mohr (1998b)	H-like $6s$ and $8d$ state SE. New results for SE screening.
Labzowsky et al. (1998a)	SE with partial-wave renormalization using B-splines. Results for H-like ns ions, Z=10-100, n=1-8.

Reference	Comments
Marrocco et al. (1998)	QED shifts of Rydberg levels between parallel metal plates.
Pyykkö et al. (1998)	Lamb shifts of ns valence electrons of neutral alkali metals Li-E119 and coinage metals Cu-E111 estimated.
Santos et al. (1998a)	$2s_{1/2} - 2p_{3/2}$ transitions of Li-like to Ne-like Bi, Th and U. Includes QED via Welton potential.
Shabaev et al. (1998a)	Recoil correction to H-like ground-state energy.
Shabaev et al. (1998b,1999)	Recoil correction to H-like energy levels.
Shabaev et al. (1998c)	QED and nuclear effects in highly charged ions.
Artemyev et al. (1999)	VP screening corrections for Li-like ions, Z=20-100.
Drake and Goldman (1999)	Bethe logarithms for Ps^-, H^-, He-like atoms.
Friar et al. (1999)	Hadronic VP and the Lamb shift.
Goidenko et al. (1999)	2nd-order SE in H-like ions. Z=3-92.
Jentschura et al. (1999)	Nonperturbative numerical evaluation of 1-photon SE for H-like ions with low Z of 1-5.
Karshenboim et al. (1999)	Analytic VP contribution to energy of H-like muonic or electronic atoms.
Kinoshita and Nio (1999)	6th-order VP contribution to Lamb shift of muonic hydrogen.
Labzowsky et al. (1999b)	Lamb shifts of ns valence electrons of neutral Li-E119, Cu-E111, Hg^+, Tl^{2+} calculated.

Table 3.4: QED: Interatomic and intermolecular interactions.

Reference	Comments
Milonni and Shih (1992b)	Casimir forces. Review.
Ford (1993)	Spectrum of the Casimir effect and the Lifshitz theory.
Iacopini (1993)	Casimir effect at macroscopic distances.
Levin and Micha (1993)	Long-range Casimir forces. Book.
F. Luo et al. (1993)	Effect of retardation on binding of He_2. R^{-7} instead of R^{-6} important.
Power and Thirunamachandran (1993)	Derive the retarded van der Waals forces between neutral molecules from vacuum-fluctuation-induced dipole moments of the monomers.
Babb and Spruch (1994)	Retardation (Casimir) potential for Rydberg H_2 from QED.
Marinescu et al. (1994a)	Interaction of two alkali atoms. Includes retardation.
Power and Thirunamachandran (1994)	Derive the fully retarded dispersion potentials, including N-body terms, N=1-4.
Spruch et al. (1994)	Asymptotic Casimir interaction of a pair of finite systems.
Jamieson et al. (1995)	Retarded dipole-dipole dispersion for He.
F. Zhou and Spruch (1995)	van der Waals and Casimir interactions of an electron or of an atom with multilayered walls.

Table 3.5: QED: High-field ionization processes.

Reference	Comments
Åberg (1993)	QED of multiphoton ionization.

Chapter 4

Multielectron Atoms: Methods

Table 4.1: General methods and basic theory for multielectron atoms.

Reference	Comments
Foldy and Krajcik (1975)	Separable solutions for directly interacting particle systems. Expansion in α^2.
Jáuregui et al. (1991)	Relativistic CI for atoms.
Crater et al. (1992); Crater and Van Alstine (1994)	Two-body interactions for spinning particles.
Lindgren (1992,1994)	Reviews on the atomic many-body problem.
Barut et al. (1993)	Relativistic two-fermion equation.
Ilyabaev and Kaldor (1993)	Relativistic coupled-cluster approach for open-shell atoms. Tested on Li, C, O, F, Na.
Indelicato and Desclaux (1993)	Projection operators needed in MCDF.
Ishikawa and Quiney (1993)	Relativistic MBPT based on DFB wave functions.
Ito and Gross (1993)	Compton scattering from relativistic composite systems.
Johnson (1993)	Relativistic MBPT on highly-charged ions.
Y.-K. Kim (1993ab)	Recent and unsettled questions in atomic structure theory.
Lindgren et al. (1993a)	Heavy-ion spectroscopy and QED in atomic systems. Symposium proceedings.
Mårtensson-Pendrill (1993a)	MBPT in atomic structure calculations.
Piekarewicz (1993b)	Salpeter's approach to the relativistic two-body problem.
Pilkuhn and Staudner (1993)	Double Dirac equation and decay rates of bound particles.
Rabinowitch (1993)	Generalization of the Dirac equation for N electrons.
Rosenberg (1993)	Derives effective Hamiltonian for a two-electron atom. Extremum principles.
Sakamoto (1993)	$N-$body bound state solution of Dirac particles in (1+1)D.
Shabaev (1993b)	A Schrödinger-like equation derived from QED for the relativistic few-electron atom.
Sommerer (1993)	Relativistic two-body wave equations.
Yokojima et al. (1993)	Derivation of Bethe-Salpeter type N-body bound state equation.
Bieroń et al. (1994)	Ground-state energy of He, He-like Ho, U, with and without negative-energy projection operators.
Boero and Cortona (1994)	Transverse exchange in DFT.
Chandra and Hess (1994)	Finite-nucleus model for DK calculations.
Darevich (1994)	Hamiltonian variational method for few-particle systems.
Froese Fischer and Jönsson (1994)	Review on MCHF atomic calculations.
Grant (1994ab,1996)	Reviews on relativistic atomic calculations.
Jáuregui et al. (1994,1996)	Relativistic atomic CI: a variational principle.
Malvetti and Pilkuhn (1994)	Equal-time relativistic two-body equations.
Mourad and Sazdjian (1994)	Two-fermion relativistic wave equations. Constraint theory. Pauli-schrödinger form.
Nagy (1994)	Relativistic DFT for ensembles of of excited states.
Applebaum (1995)	Fermion stochastic calculus in Dirac-Fock space.
Broyles (1995)	Derives the Dirac-Breit Hamiltonian.
Devine and Wallace (1995)	Instant two-body equation in Breit frame.
Indelicato (1995)	Projection operators in MCDF calculations. Applied on ground states of He-like atoms.
Kenny et al. (1995)	QMC correlation and Breit energies for He-like systems, Be and Ne. Mass-polarization included.

Reference	Comments
Lindgren et al. (1995b)	Few-body problems in atomic physics.
Pilkuhn (1995)	An M1 hyperfine operator between two Dirac particles, both having anomalous magnetic moments.
Dzuba et al. (1996bc)	MBPT method for more than one valence electron.
Essén (1996)	Review derivation of the Darwin Lagrangian. Macroscopic consequences of the magnetic part.
Evans et al. (1996)	The spectrum of the electron equation by Bethe and Salpeter.
Häckl and Pilkuhn (1996)	Transformation of Breit operators into hyperfine-like operators.
Indelicato (1996)	Correlation and negative continuum effects for the M1 transition in two-electron ions. MCDF.
Kolakowska et al. (1996)	Minimax variational approach to relativistic two-electron problem.
Lindgren (1996)	Relativistic many-body and QED calculations on atomic systems.
Parpia et al. (1996)	The GRASP92 atomic MCDF package.
Phillips and Wallace (1996)	Derive a 3D bound-state equation from the 4D Bethe-Salpeter one for two-body boson or fermion systems.
L.-J. Wu (1996)	R MBPT including 'pseudoconfigurations'. Be ground state.
Badnell (1997)	Two-body, non-fine-structure operators (contact spin-spin, two-body Darwin, orbit-orbit) incorporated into AUTOSTRUCTURE code.
Bijtebier (1997); Bijtebier and Broekaert (1997)	Solutions of the Bethe-Salpeter equation.
Cea (1997)	Vacuum stability for 3D fermions problem for large m.
Ishikawa et al. (1997)	Finite-nucleus models for GTO spinors.
Jáuregui et al. (1997ab)	Eigenvalue spectra of the 'no pair' Hamiltonian. Tests on 1- and 2-electron systems.
Jáuregui et al. (1997c)	Buildup of many-electron atoms from QED.
Y.-K- Kim (1997)	Review on relativistic atomic structure calculations.
King (1997,1999)	High-precision calculations on the Li atom. Review.
Kołakowska (1997)	Explicitly correlated (r_{12}), Hylleraas-type relativistic wave functions for He-like systems.
Bunge et al. (1998ab)	Decoupling of positive- and negative energy states.
Entralgo et al. (1998)	The problem of two point particles with spin.
Feldmann et al. (1998)	S states of 3-electron atoms. BP Hamiltonian and explicitly correlated wave functions lead to individual divergencies which, however, cancel.
Y.-K. Kim et al. (1998)	Failure of MCDF at NR limit. The wave function for specific J may not reduce to the LS limit. Possible remedies discussed.
Klink (1998ab)	Relativistic QM for particles, each of which is a bound state of a mass operator.
Lindgren (1998)	Review on electron correlation and QED.
Long and Crater (1998)	Two-body Dirac equations for general covariant interactions. Their coupled Schrödinger-like forms.
Lucenti et al. (1998)	Dirac observables and spin bases for N particles.
I. Martin (1998)	Relativistic quantum defect orbital method.
Monahan and McMillan (1998)	Faddeev equation for relativistic two- and three-body system.

Reference	Comments
Reiher (1998)	Numerical algorithms for MCDF. Thesis.
Ruijgrok (1998)	General requirements for a relativistic quantum theory for two or more particles. Quasipotential theory recommended.
Sigg and Sorg (1998)	Nature of exchange terms in a two-particle relativistic Schrödinger theory. A potential.
Sucher (1998)	What is the force between the electrons? Searches an effective electron-electron potential.
Sunnergren (1998)	Symmetrical spectrum method to avoid fermion doubling.
Dürr et al. (1999)	'Hypersurface Bohm-Dirac models.' N entangled but noninteracting Dirac particles.
Esteban and Séré (1999)	Claim, from a mathematical point of view, that the DF equations have infinitely many solutions.
Lindgren (1999)	QED effects in strong nuclear fields. Review.
Noyes and Jones (1999)	Relativistic three-body problem. Only the masses m_a, m_b, m_c defined.
Reiher and Hinze (1999)	Self-consistent treatment of the Breit term in MCDF.
Sapirstein et al. (1999)	Potential-independence in relativistic MBPT achieved if negative-energy states are included. He-like ions. 'No-pair' not enough.

Table 4.2: Published programs for atoms.

Reference	Comments
Eissner (1991b)	SUPERSTRUCTURE. A BP-level atomic code.
Parpia et al. (1993)	Complete active spaces (CAS) for atomic calculations.
Perger et al. (1993)	Continuum solver for the GRASP code.
Salvat and Mayol (1993)	Partial wave analysis for electron and positron elastic scattering.
Young and Norrington (1994)	Solution of relativistic asymptotic equations in electron-ion scattering.
Berrington et al. (1995)	RMATRIX I. The Belfast atomic R-matrix code.
Fritzsche and Grant (1995); Fritzsche (1997)	Expansion of jj-coupled symmetry functions into determinants.
Kroger and Kroger (1995)	Program for angular coefficients of relativistic one-electron hfs parameters.
Szmytkowski (1995)	Relativistic multi-channel variable phase program for asymptotic equations of electron-atom and electron-ion scattering.
Ankudinov et al. (1996)	Single-configuration version of the DF code of Desclaux (1975).
Jönsson et al. (1996)	HFS92: A program for atomic hfs calculations. MCDF.
Parpia et al. (1996)	The GRASP92 atomic MCDF package.
Pöschl et al. (1996); Pöschl (1997,1998)	B-spline finite-element codes. Primarily for nuclear problems.
Jönsson and Froese Fischer (1997)	SMS92: Relativistic isotope shift calculations.
Fritzsche et al. (1999)	Expansion package RATIP for GRASP92 for various transition and ionization properties.
Chernysheva and Yakhontov (1999)	A DF code. Continuum states and muons can be included.
Fuchs and Scheffler (1999)	PP for polyatomic systems from SR DFT theory.

Table 4.3: Numerical four-component methods.

Reference	Comments
Froese Fischer and Parpia (1993)	Accurate spline solution of radial Dirac equations.
Sapirstein and Johnson (1996)	Use of splines in atomic physics.
Sapirstein et al. (1999)	Potential-independence in relativistic MBPT achieved if negative-energy states are included. He-like ions. 'No-pair' not enough.

Table 4.4: Four-component approaches for many-electron atoms..

Reference	Comments
Da Silva et al. (1993ab)	Universal Gaussian basis set for DF calculations.
Gambhir and Ring (1993)	Solution of Dirac equation using GTO basis for nuclei. Recipe for avoiding spurious states.
Ley-Koo et al. (1993)	Two-body integrals for relativistic atomic calculations. Both Coulomb and Breit.
Malli et al. (1993ab, 1994)	Universal Gaussian basis for DF calculations.
Koc and Ishikawa (1994)	Single-Fock-operator method for DF on open-shell atoms. Li-K, B-In.
Koc et al. (1994)	Relativistic CI calculations on open-shell atoms.
S. N. Datta (1995)	DFB tests on He-Ne.
Minami and Matsuoka (1995)	GTO basis for $_{86}$Rn-$_{94}$Pu. DF.
Deineka (1996)	B-spline methods.
Dzuba et al. (1996bc)	MBPT method for more than one valence electron. Combination of MBPT and CI.
Jorge et al. (1996,1997ab); Jorge and da Silva (1998)	GTO-basis sets.
Jorge and da Silva (1996ab,1997)	Generator coordinate DFB.
Koc et al. (1996)	Relativistic modification of asymptotic CI. C-like systems, $Z \leq 106$.
Ley-Koo et al. (1997)	Relativistic atomic r_{12}^{-1} integrals using perimetric coordinates.
Vilkas et al. (1997)	2nd-order MRCI based on MCDF functions.
Visscher and Dyall (1997)	DF atomic calculations using different nuclear charge distributions. Z=1-109.
Malli and Ishikawa (1998)	Geometric series of Gaussian exponents from 'generator coordinate DF method' for open-shell atoms.
Vilkas et al. (1998b)	Relativistic MR MP method based on MCDF reference functions.
Chaudhuri et al. (1999a)	GTO-basis MBPT.
Vilkas et al. (1999)	Relativistic MR MBPT for quasidegenerate systems.

Table 4.5: Relativistic density functional theory.

Reference	Comments
Dreizler (1993)	Relativistic DFT.
Holas and March (1993)	Relativistic DFT reduced to the Dirac equation.
March (1993)	Completely local, relativistic DFT. Role of the virial. Applied to Thomas-Fermi theory and heavy atoms in magnetic fields.
Nagy (1994)	Relativistic DFT for ensembles of of excited states.
Rajagopal (1994)	DFT including EM fields in condensed matter.
Engel (1995); Engel and Dreizler (1996)	Reviews on relativistic density functional theory.
Engel et al. (1995)	Local and non-local relativistic exchange-correlation functionals.
Rieger and Vogl (1995)	Relativistic self-interaction-free DFT.
Vijayakumar and Gopinathan (1995)	Atomic tests of the authors' Ξ functional. Relaxation effects, Koopmans' theorem discussed.
Engel et al. (1996)	GGA for relativistic exchange-only energy functional.
E. K. U. Gross et al. (1996)	DFT of time-dependent phenomena.
Kenny et al. (1996)	QMC for relativistic homogeneous electron gas. PT relativity.
Rajagopal and Buot (1996)	Fundamentals of time-dependent DFT, including EM fields.
Engel et al. (1997)	Relativistic corrections to exchange-correlation functional.
Higuchi and Hasegawa (1997, 1998)	Relativistic current- and spin-density functional theory. Applications on Ln^{3+} ions; Ln=Ce-Yb.
Engel et al. (1998)	Relativistic optimized potential method for DFT. Exact transverse exchange and MPn-based correlation potential. No-pair gives gauge independence.
Facco Bonetti et al. (1998)	Relativistic exchange-correlation energy functional. Gauge dependence of no-pair correlation energy.
Grabo et al. (1998)	Optimized effective potential DFT. Review.
Kreibich et al. (1998)	Approximate relativistic optimized potential method.
W.-J. Liu and Dolg (1998)	IPn and $d-f$ transitions of La-Yb; n=1-4. Several density functionals compared with QR PP.
W.-J. Liu et al. (1998c)	IPn; n=1-4, $5f-6d$ excitation energies of Ac-No. DFT and PP methods compared.
Tong and Chu (1998)	Relativistic DFT with self-interaction correction. Right $(-1/r)$ long-range behaviour. Atomic ground states, Z=2-106.
Engel and Dreizler (1999)	DFT that claims to include van der Waals effects.
Eschrig and Servedio (1999)	DFT approach to open-shell atoms (C-Pb + ions).
Schmid et al. (1999)	Relativistic GGA tested on $5d$ TM. Band structure and cohesive properties. Relativity changes exchange at 1% level, is negligible for correlation functional.

Table 4.6: Thomas-Fermi calculations.

Reference	Comments
March (1993)	Completely local, relativistic DFT. Role of the virial. Applied to TF theory and heavy atoms in magnetic fields.
Shivamoggi and Mulser (1993)	Relativistic TF model for atoms in a strong magnetic field.
Shivamoggi (1995)	Relativistic TF theory with thermal effects, with or without a very strong magnetic field.
Lieb et al. (1996)	Stability of relativistic matter via TF theory. Finds stability for $Z \leq 59$ if $\alpha = 1/137$.
March (1997)	TF theory and $1/Z$ expansions for large Z.

Table 4.7: Independent-particle models.

Reference	Comments
J.-J. Chang (1993,1998)	Dirac quantum-defect theory.
U. I. Safronova et al. (1993)	Screening theory for transition energies of highly charged ions.
Stein (1993)	A local, 1-VE PP for Li-Cs atoms. Tested on $s - f$ states.
Bielinska-Waz et al. (1994)	Core-polarization effects in the relativistic quantum-defect-orbital theory.
Nana Engo et al. (1997)	Supersymmetry-inspired R and QR quantum-defect theory. Applications on transition matrix elements.
Schweizer et al. (1999)	Local model potential for Li-Cs and Li-like ions, Z=3-10.

The following Table 4.8 contains the methodological developments, including the new pseudopotentials, since RTAM II. No distinction has been made between between the pseudopotentials with nodeless pseudo wavefunctions, and the 'model potentials' whose wave functions contain the nodes. For a steady update of the Stuttgart energy-consistent PP, see *http://www.theochem.uni-stuttgart.de/*.

Table 4.8: Pseudopotentials: Methodological work.

Reference	Comments
Stevens et al. (1984)	PP for Li-Ne, Na-Ar. (NR.)
Igel-Mann (1987)	PP for main-group and d^{10} TM elements.
Vanderbilt (1990)	Soft self-consistent PP.
Gonze et al. (1991)	Analysis of separable pseudopotentials.
Troullier and Martins (1991)	PP for plane-wave calculations. R/NR for Z<72, some Z>72.
Kaupp (1992)	PP applications. Thesis.
Bergner et al. (1993)	Energy-consistent PP for Groups 13-17 (B-In, .. F-I).
Cundari and Stevens (1993)	PP for Ce-Lu. Pd-like (46-e) core.
Czuchaj et al. (1993)	Ne-Xe, Ba PP.
Dolg et al. (1993c)	Energy-consistent PP for Ha (element 105). SO.
Ehlers et al. (1993)	An f-polarization function for $3d, 4d, 5d$ TM PP. Optimized for the CISD energy of the lowest s^1d^n state.
Häussermann et al. (1993)	Energy-consistent R/NR PP for Hg.
Hemstreet et al. (1993)	SO PP for solids. III-V semiconductors.
Höllwarth et al. (1993)	A d-type polarization function for main-group B-Bi. An f-polarization function for Zn-Hg.
Leininger et al. (1993)	MH^+, M=Fe-Os. Compare several PP.
Marino and Ermler (1993)	Core-valence correlation potential operator. Cs.
Stein (1993)	A local, 1-VE PP for Li-Cs atoms. Tested on $s-f$ states.
Ermler and Marino (1994,1996)	Review on PP methods.
Fernandez Pacios and Gomez (1994)	Triple-zeta GTO basis for PP.
Kresse and Hafner (1994)	Norm-conserving and ultrasoft PP for first-row and transition elements.
Küchle et al. (1994)	PP for Ac-Lr. SO potential included.
Mitas (1994)	PP QMC calculation of IP and EA of Fe.
Ross et al. (1994)	PP for Ln, Ce→Lu. 54-e core. SO.
Shukla and Banerjee (1994)	A four-component relativistic DF method for valence electrons only. An effective core-valence potential constructed. Tested on atoms, Li-S.
Casarrubios and Seijo (1995)	Test of WB MP on Pt.
Huzinaga (1995)	Review on 'active electrons in chemistry'.
Koseki et al. (1995)	Effective Z for SO splitting using Stevens' pseudo wave functions.
Nicklass et al. (1995)	R/NR PP for Ne-Xe. SO.
Schwerdtfeger et al. (1995a)	Accuracy of the PP approach tested on InCl, $InCl_3$.
Seijo (1995)	Derive PP including SO part from the WB Hamiltonian. F-At, Tl→Rn.
Titov and Mosyagin (1995)	New PP for Cu-Au.
Tuan and Pitzer (1995a)	PP for Hf.
Tupitsyn et al. (1995)	'Generalized ECP:s' for Hg→Bi. Atomic tests only.
Wittborn and Wahlgren (1995)	New PP for $5d$ metals.
Charpentier et al. (1996)	PP including semicore for Ba, Ce, Th. Plane wave basis.

Reference	Comments
Cundari et al. (1996)	Review on pseudopotential methods.
Dolg (1996a)	Energy-consistent 1-VE PP for Group 1 (Li-Cs).
Dolg (1996bc)	Accuracy of the 7-VE energy-consistent PP for Group 17 tested. Differential effects of the nodelessness are small.
Frenking et al. (1996,1999); Frenking and Pidun (1997)	Reviews on transition-metal compounds.
Gordon and Cundari (1996)	Pseudopotential studies on transition-metal compounds. Review.
Kaupp (1996e)	PP applications on TM systems. Habilitation.
Leininger et al. (1996a)	9-VE PP for K-Cs.
Leininger et al. (1996b)	13-VE and 21-VE PP for In.
F. Nogueira et al. (1996)	Transferability of *local* PP, based on solid-state electron density.
Blaudeau and Curtiss (1997)	Basis sets for the PP of K, Ca, Ga-Kr. PP of Hurley et al. (1986) used.
Eichkorn et al. (1997)	Auxiliary basis sets for Z = 1-56, 72-85. RI method.
Flad and Dolg (1997)	Accuracy of PP for TM in MC calculations. Sc→Cr. IP within 0.1 eV.
Flad et al. (1997)	SO coupling in variational MC calculations. Pb, Bi^+, Po^{2+}.
Leininger et al. (1997)	R/NR 13-VE and 21 VE PP for Ga, Tl.
Menchi and Bosin (1997)	DFT PP in QMC.
Mosyagin et al. (1997)	Generalized PP for Hg-Tl. Claims higher accuracy. Has many parameters.
Nash et al. (1997)	PP for $_{95}$Am-(E118). SO also given.
Pollack et al. (1997)	Density-based local PP for 16 simple metals.
Sakai et al. (1997)	PP for main-group elements, Li-Rn.
Seth et al. (1997)	PP for E111 and E112.
Wildman et al. (1997)	New PP for Tl→Rn. $5d6s6p$ valence shells. Special consideration on f shells.
Buenker et al. (1998)	SO splittings and PP. Tl ground state as example.
Casarrubios and Seijo (1998)	WB-based MP for B-Ba (Z = 5-56).
Decker et al. (1998)	Calibration of model potentials for main-group elements. N_2-Sb_2, F_2-I_2, XY (X=C-Sn, Y=O-Te), OH_2-TeH_2, NH_3-SbH_3, ...
Delley (1998)	Scattering-theory approach to scalar relativistic corrections to bonding. Local pseudopotential can include them.
Féret and Pascale (1998)	Two electrons in a PP. Ba.
Hartwigsen et al. (1998)	'Separable dual-space Gaussian PP' for H-Rn. LDA.
Y. S. Kim et al. (1998)	Kramers-unrestricted molecular PP calculations at HF or MP2 level. SO PP used.
W.-J. Liu and Dolg (1998)	IPn and $d-f$ transitions of La-Yb; n=1-4. Several density functionals compared with QR PP.
W.-J. Liu et al. (1998c)	IPn; n=1-4, $5f-6d$ excitation energies of Ac-No. DFT and PP methods compared.
Miyoshi et al. (1998)	PP for main-group elements Ga-Kr, In-Xe, Tl-Rn.
Rakowitz et al. (1998)	Ir^+. A new SO operator tested.
Sakai et al. (1998)	PP for Ln (La-Lu). 46-e core.
Sanoyama et al. (1998)	Low-lying levels of Ln^{3+}; Ln=Ce-Eu, Tb-Yb. Compare different PP. Semi-core correlation ($4d, 5s, 5p$) important.
Schautz et al. (1998)	2-VE PP for Zn-Hg.
Schimmelpfennig et al.	The 'atomic-mean-field integral (AMFI)'

Reference	Comments
(1998ab)	approach to SO CI. Tested on the Pt atom.
Seth (1998)	PP for E111-E120.
Y. X. Wang and Dolg (1998)	10-VE ($5s5p6s$) PP for Yb.
Alatalo et al. (1999)	Truncated pseudopotentials for alloy calculations. Cut-offs in momentum space introduced. Pd-Al alloys as example.
Casarrubios and Seijo (1999)	WB-based MP for La, Hf-Hg (Z = 57,72-80). V_{SO} included.
Fuchs and Scheffler (1999)	PP for polyatomic systems from SR DFT theory.
Rakowitz (1999)	Development of PP methods, especially for SO. Thesis.
Rakowitz et al. (1999ab)	PP for TM, Sc to Hg.
Ramer and Rappe (1999)	Nonlocal PP with improved transferability. H,Si,Ca,Zr,Pb.
Titov and Mosyagin (1999)	'Generalized Relativistic ECP'. Many further parameters give moderate increase in accuracy in atomic tests.
Trail and Bird (1999a)	Core reconstruction in PP calculations. Full Dirac.
Trail and Bird (1999b)	Uses this method for calculating structure factors.

The Table 4.9 contains the available references on atoms in strong laser fields. No complete coverage is attempted. Some of these references also appear in other tables.

Table 4.9: Atoms in strong laser fields.

Reference	Comments
Faisal and Radozycki (1993)	3D model for bound particle in laser pulse.
Ovcharov and Fedosov (1993)	Correlated coherent states of electron in field of plane EM wave.
Radozycki and Faisal (1993)	Multiphoton ejection of strongly bound relativistic electrons.
Rosenberg and Zhou (1993)	Dirac and KG particles in a multimode laser field: Generalized Volkov solutions.
Keitel (1996)	Ultra-energetic electron ejection in relativistic atom. Laser field interaction.
Meyerhofer et al. (1996)	Relativistic mass-shift effects during high-intensity laser–electron interactions. Multiphoton scattering.
Ehlotzky et al. (1997)	Electron–atom collisions in a laser field.
Kylstra et al. (1997)	1D model atom in intense laser field.
Protopapas et al. (1997)	Atomic physics with super-high intensity lasers. Review.
Rathe et al. (1997)	Intense laser-atom dynamics with 2D Dirac equation.
Szymanowski et al. (1997)	Relativistic calculation of two-photon bound-bound transition amplitudes in hydrogenic atoms.
Crawford and Reiss (1998)	Relativistic ionization of hydrogen by linearly polarized light.
Goreslavsky and Popru-shenko (1998)	Relativistic deflection of photoelectron trajectories in elliptically polarized laser fields.
Krainov (1998)	Energy distribution of relativistic electrons in the tunneling ionization of atoms by super-intense laser radiation.
Matrasulov (1998,1999)	Chaotic ionization of an H-like atom in intensive mono-chromatic field.
Reiss (1998)	Introduction to special issue on 'Relativistic effects in strong electromagnetic fields. After low-field E1, next comes 'figure-8' pattern due to magnetic component. Full relativistic effects when the kinetic electron energy approaches mc^2.
Q. Su et al. (1998)	Relativistic suppression of wave packet spreading.
Szymanowski and Maquet (1998)	Relativistic signatures in laser-assisted scattering at high field intensities.
Taïeb et al. (1998)	Signature of relativistic effects in atom-laser interactions at ultrahigh intensities. 1D 'soft-core Coulomb' model: $V(x) = -q/\sqrt{2+v^2}$. KG.
J.-H. Wen et al. (1998)	High harmonics of H atom in ultrastrong laser field. MC.
Yu and Takahashi (1998)	Dirac electron in two-frequency circularly polarized EM wave. Radiation and pair production.
J. Chen et al. (1999)	High-order harmonics for H-like atom in ultrastrong laser field.
Krainov (1999)	Energy and angular distribution of relativistic electrons in the tunnelling ionization of atoms by circularly polarized light.
Panek et al. (1999)	Angular and polarization effects in relativistic potential scattering of electrons in a powerful laser field.
Soliman and Abelraheem (1999)	Modification of band structure in intense laser fields. 1D model. New gaps introduced.

Table 4.10: $1/Z$ and other similar expansions for many-electron atoms.

Reference	Comments
Shabaeva and Shabaev (1995)	Interelectronic contribution to hfs of Li-like ions. $1/Z$ expansion, including QED effects. Z=5-100.
Weiss and Kim (1995)	Relativistic modifications of charge expansion theory. Introduce shells with same (nj).
March (1997)	Thomas-Fermi theory and $1/Z$ expansions for large Z.
Yan et al. (1998)	$1/Z$ extrapolations for $2s$ and $2p$ states of Li-like systems.
Safronova and Shlyaptseva (1999)	Autoionization rates and energies for C-, N-, O-, and F-like ions with $Z = 6 - 54$. $1/Z$ expansion.

Table 4.11: Related nuclear calculations.

Reference	Comments
Centelles et al. (1993)	Semiclassical nuclear mean-field theory.
Fritz et al. (1993)	Dirac effects in HF calculations on finite nuclei employing realistic forces. Increase the binding energy *and* the charge radius for ^{16}O and ^{40}Ca.
Gambhir and Ring (1993)	Solution of Dirac equation using GTO basis for nuclei. Recipe for avoiding spurious states.
Yokojima et al. (1993)	Derivation of Bethe-Salpeter type N-body bound state equation.
Fearing et al. (1994)	Compare the FW and Pauli approximations in nuclear physics. FW found better.
Warrier and Gambhir (1994)	SO splitting in relativistic nuclear mean field theory.
Zamick and Zheng (1994)	Nuclear structure with Dirac phenomenology.
Forest et al. (1995)	Relativistic nuclear Hamiltonians. Combines two- and three-body potentials in rest frame with boosts.
Nefiodov et al. (1996)	Nuclear polarization effects on spectra of multicharged ions. H-like ^{208}Pb, ^{238}U. Effects small.
Phillips and Wallace (1996)	Derive a 3D bound-state equation from the 4D Bethe-Salpeter one for two-body boson or fermion systems.
Pöschl et al. (1996); Pöschl (1997,1998)	B-spline finite-element codes. Primarily for nuclear problems.
Bijtebier (1997); Bijtebier and Broekaert (1997)	Solutions of the Bethe-Salpeter equation.
Ring (1997)	Relativistic mean-field program for even-even nuclei.
Stoitsov et al. (1997)	Relativistic nuclear calculations using a transformed harmonic-oscillator basis.
Klink (1998ab)	Relativistic QM for particles, each of which is a bound state of a mass operator.
Tomaselli et al. (1998)	M1 $1s$ hfs in H-like atoms with one-hole nuclei. ^{165}Ho...^{207}Pb.
Blum and Brockmann (1999)	Dirac sea effects and the stability of nuclear matter.

Chapter 5

Multielectron Atoms: Results

Table 5.1: Tabulations of atomic ground-state properties.

Reference	Comments
Chakravorty et al. (1993)	Atomic ground-state energies for 3-18 electrons, Z=3-36, .. Includes Dirac-Breit +QED.
García de la Vega and Miguel (1994)	Momentum expectation values, $\langle p^n \rangle$, n = -2 to +4 for atomic ground states, Cs, U. DF/HF.
Ishikawa and Koc (1994)	Ground states of Ne-Rn, Zn-Hg, Ne-like ions.
Indelicato (1995)	Projection operators in MCDF calculations. Applied on ground states of He-like atoms, Z=10-100.
Kenny et al. (1995)	QMC relativistic and Breit corrections for He-like systems, Be and Ne. Much smaller Breit contributions than at DF level.
Ishikawa and Koc (1996)	Li-like systems, $Z \leq 20$.
Kotochigova et al. (1996,1997)	LDA ground-state energies for atoms 1-92.
Cioslowski et al. (1997)	MCDF core-electron densities, Z=3-118.
Forstreuter et al. (1997)	Ln atoms and ions. Ln=Ce→Lu. DFT tested.
King (1997,1999)	High-precision calculations on the Li atom. Review.
King et al. (1998)	Hylleraas-type calculation of BP relativistic corrections for the Li ground state.
Frolov (1999)	Ground-state properties of the positronium anion, Ps^-. BP.

Table 5.2: Energy levels.

Reference	Comments
Y. Zhang et al. (1992b)	Na-like Nb.
Arp et al. (1993)	K-shell spectra of Ca, Cr, Mn, Cu. $1s \rightarrow 4p$ important.
Berry et al. (1993)	QED and $1s2s$ - $1s2p$ triplet state energies of He-like systems, Z=2-92.
Berseth and Darewych (1993)	Relativistic corrections to Ps^-.
Birkett et al. (1993)	$2\ ^3P_0$–$^3P_1$ FS splitting of He-like Ag. Hyperfine quenching.
M.H. Chen et al. (1993)	$n = 2$ triplet states of He-like ions, Z=5-100.
X.-L. Cheng et al. (1993)	Ni-like ions, $47 \leq Z \leq 54$.
Chevary (1993)	Ground-state DF configurations for M^-, M=Sr-Ra,Yb,La,Lu.
Chou et al. (1993ad)	Hg-like ions,
Chou et al. (1993bd)	Cd-like ions.
Chou et al. (1993c)	Mg-like ions.
K. T. Chung and Zhu (1993)	$2snl$ states of the Be atom. FS, isotope shifts.
Connerade et al. (1993)	Rydberg levels for alkali metals.
Drake (1993c)	Review on He Rydberg levels.
Harra et al. (1993)	He-like Ni. $1s2l$, $1s3l$. MCDF.
Ilyabaev and Kaldor (1993)	Relativistic coupled-cluster approach for open-shell atoms. Li, C, O, F, Na.
Kronfeldt et al. (1993b)	Fine and hyperfine structure of Er I, $4f^{11}5d6s6p$.
Liaw (1993b)	Alkali metal atoms in the Brueckner approximation.
C. D. Lin (1993)	Classification and properties of doubly excited states.
Lindroth and Indelicato (1993,1994)	Inner-shell transitions in heavy atoms.
Marketos et al. (1993)	O III excitation energies.
Marques et al. (1993a)	Hyperfine quenching of Be-like $1s^22s2p\ ^3P_0$.
Marques et al. (1993b)	Hyperfine quenching of Mg-like $3s3p\ ^3P_0$.

Reference	Comments
I. Martin et al. (1993)	Li-like sequence. QDT.
Migdalek and Stanek (1993)	$5s^2 - 5s5p$ transitions in the Sr sequence.
Rath and Patnaik (1993)	$2p$ SO splitting of Li-like systems.
U. I. Safronova et al. (1993)	Screening theory for transition energies of highly charged ions.
Shabaev (1993a)	Finite-nuclear-size corrections to energy levels of multicharged ions. Expressed in terms of nuclear $\langle r^n \rangle$; n=2,4. Z=1-100.
Simionovici et al. (1993)	$n = 3$ transitions of Na-like Pb.
Trigueiros et al. (1993)	$4p^4$ configuration of Ge-like Kr V.
Verner et al. (1993)	Subshell ionization energies of He-Zn.
Vidolova-Angelova (1993)	Sr I.
Vosko and Chevary (1993)	Electron shell filling of Ln anions: Lu^- is $5d^16s^26p^1$.
P. Wang et al. (1993)	Kα satellites of Al. BP.
W. J. Wang (1993)	FS levels in N-like Co-Zn. MCDF.
Z. W. Wang et al. (1993)	$1s^2np$ states; n=2-5 for Li-like systems.
L. Yang (1993)	K-shell excitation and ionization of Na.
Zilitis (1993)	Rydberg levels of Li-like ions, Z=3-16.
Anisimova et al. (1994)	Two-el. atoms with p and d electrons.
Biémont et al. (1994a)	Resonance transitions of Cl.
Bieroń et al. (1994)	Ground-state energy of He, He-like Ho, U, with and without negative-energy projection operators.
M.-K. Chen and Chung (1994)	Core-excited doublet states of Li.
K. T. Cheng et al. (1994)	Singlet states for He-like ions, $n = 2$, $4 \leq Z \leq 92$.
X.-L. Cheng et al. (1994)	Ni-like ions, $72 \leq Z \leq 79$.
Chevary and Vosko (1994)	Ground-state configuration for Tm^-.
Chou et al. (1994a)	Zn-like ions.
Chou et al. (1994b)	Be-like ions.
Dembczynski et al. (1994)	Odd-parity levels of Pb I.
Dzuba et al. (1994)	Dy.
Eliav et al. (1994a)	Au^+, Au. DFB+CCSD.
Eliav et al. (1994b)	Ground states of atoms with 2-5 electrons. DFB+CCSD.
Eliav et al. (1994c)	Li-Fr. DFB+CCSD.
Eliav et al. (1994d)	Xe ground-state energy and pair correlations.
Eliav et al. (1994e)	E111 (eka-Au). Ground state d^9s^2, not $d^{10}s^1$.
Flambaum et al. (1994)	Chaotic spectrum of Ce.
Fritzsche and Grant (1994a)	P II $^5S_2 - ^3P_J$ intercombination transitions.
Fritzsche and Grant (1994b)	Be-like ions, $2s^2\ ^1S_0$-$2s3p\ ^3P_1$ intercombination transitions.
Froese Fischer (1994)	C II and C III.
Gaigalas et al. (1994)	O isoelectronic sequence.
Gębarowski et al. (1994)	$3s^23p - 3s^23d$ transitions for Al-like sequence.
Gleichmann and Hess (1994a)	Hg at DK MRCI level.
Haftel and Mandelzweig (1994a)	Rel., finite-size and QED corrections for the $2\ ^1S$ state of He.
Haftel and Mandelzweig (1994b)	He ground state.
Hsu et al. (1994)	^4P series of Li. Autoionization.
Itoh et al. (1994)	Relativistic effects on multiplet terms of lanthanide ions.
Lindroth (1994)	Doubly excited states of He with a finite, discrete spectrum.

Reference	Comments
Pershina et al. (1994b)	Energy levels of M^{q+}; M=V-Db(E105); q=0, 5.
Plante et al. (1994)	n=1,2 states of He-like ions, Z=3-100.
U. I. Safronova (1994)	$2p^{-1}nl$ and $2s^{-1}nl$ levels of Ne-like ions. Z=20-60, n=3-6, l=0-3.
U. I. Safronova and Bruch (1994)	Transition and Auger energies of Li-like ions. $1s2lnl'$ configurations.
U. I. Safronova et al. (1994a)	$1s2s^22p^n$ and $1s^22s^22p^n$ configurations as function of Z. Compares the SUPERSTRUCTURE and MZ codes.
U. I. Safronova and Nilsen (1994)	Autoionization states of Li-like ions with large n.
U. I. Safronova et al. (1994b)	Ne-like ions, $2p^{-1}nl$, $2s^{-1}2p^{-1}nl$, $n = 3-6$, $l = 0-3$. Z=20-60.
U. I. Safronova et al. (1994c)	Two-electron doubly-excited states.
Shabaev and Artemyev (1994)	Relativistic nuclear recoil corrections for multicharged ions.
Tolstikhina et al. (1994)	K x-ray satellite energies for Ar^{17+} upon metallic surface.
Vilkas et al. (1994)	O-like sequence.
Ynnerman et al. (1994)	$2p - 2s$ energies in Li-like U.
Zilitis (1994)	Al-like ions.
Anisimova et al. (1995)	Ne $2p^5nd$ levels, n=3-8.
Avgoustoglou and Beck (1995)	Ne-like $2p^53s$ levels, Z = 10-92.
M. H. Chen et al. (1995)	$n = 2$ states of Li-like ions.
Connerade et al. (1995)	Level statistics in complex spectra.
Datta and Beck (1995)	FS of ^{139}La II, $(5d + 6s)^2$.
Dzuba et al. (1995)	Fr.
Eliav et al. (1995a)	Rf (E104) ground state $7s^26d^2\ ^3F_2$. DFB+CCSD.
Eliav et al. (1995b)	The f^2 Pr^{3+} and U^{4+}. DFB+CCSD.
Eliav et al. (1995c)	Yb, Lu, Lr. Ground state of Lr(E103) $7s^27p_{1/2}\ ^2P_{1/2}$.
Eliav et al. (1995d)	Hg, E112 (eka-Hg). Ground states of the latter mono- and dication d^9s^2 and d^8s^2, respectively.
Fritzsche et al. (1995)	Cl-like ions, $3p^43d$ configurations.
Gribakina et al. (1995)	The Ce atom as a 'chaotic' system. Recall Flambaum et al. (1994).
W. Huang et al. (1995)	Ne I excited levels.
Johnson et al. (1995)	$2s_{1/2} - 2p_{3/2}$ transitions in Li-like to Ne-like U. Includes one-loop QED corrections.
Komninos et al. (1995)	^2D level of Al.
Kornienko et al. (1995)	Effect of CI on SO parameter of Ln ions.
Kukla et al. (1995)	He-like Ar^{16+}, $1s2s\ ^3S - 1s2p\ ^3P$. Uncalculated QED terms estimated as $0.15(Z\alpha)^4$ a.u.
Liaw (1995)	Bound states of Ca^-. No EA in Brueckner approximation.
Y. Liu et al. (1995)	Photoexcitation of Ni $3p$ level. SO, exchange, hybridization.
Mårtensson-Pendrill et al. (1995)	Low-Z $1s2p$ states of He-like systems.
I. Martin et al. (1995)	Ag I isoelectronic sequence. QDT.
Neale and Wilson (1995)	Influence of core polarization on FS splittings of Kr VIII. MCDF.
Pal'chikov and von Oppen (1995)	Spin-spin mixing of $1s3s\ ^3S_1$ and $1s3d\ ^3D_1$ states in the He-like sequence. Z=2-100.

Reference	Comments
Polasik (1995)	$K\beta_{1,3}L^0M^r$ x-ray spectra of Mo, Pd, La. MCDF.
Wijesundera et al. (1995)	Ground state of Lr. MCDF.
Yan and Drake (1995)	$2s$, $2p$ and $3d$ levels of Li.
H. Y. Yang and Chung (1995)	Be-like systems, $Z = 3 - 10$, core-excited $1s2s2p^2(^2P)$ and $1s2p^3(^5S)$ states.
Ynnerman and Froese Fischer (1995)	Be-like systems, Z=6...42. The E1 $2s^2\ ^1S_0 - 2s2p\ ^1P_1$ and the forbidden $2s^2\ ^1S_0 - 2s2p\ ^3P_1$ energies and TP.
Zilitis (1995)	$3p$, $3d$ levels of Al-like systems. Several crossings, non-monotonical $3d$ FS splittings.
Aspromallis et al. (1996)	Be^- $1s^22s2p^2\ ^4P$ fine structure.
Avgoustoglou and Liu (1996)	Ne-like $[2p^53d]_{J=1}$ levels, Z = 10-92.
Aymar et al. (1996)	Review on multichannel Rydberg spectroscopy.
Charro et al. (1996)	Triplet-triplet transitions in Be-like ions.
K. T. Cheng and Chen (1996)	$2s - 2p_{3/2}$ transitions in Li-through-F-like U.
Chou et al. (1996)	S-like ions, $Z \geq 18$.
Dzuba et al. (1996bc)	Tl.
Eliav et al. (1996a)	Ba, Ra. NR ground states of both cations are d^1, not s^1. Relativistic M^+ are s^1.
Eliav et al. (1996c)	Tl, E113 (eka-Tl). Low-lying $6d$ hole states found. 'Is eka-Tl a transition element?'
Indelicato (1996)	Correlation and negative continuum effects for the M1 transition in two-electron ions. MCDF.
Ishikawa and Koc (1996)	Li-like systems, $Z \leq 20$.
Ivanov and Ivanova (1996)	Sturmian orbital method for radiation physics of atoms and ions. $2l3l$, $2l4l$ levels of Ne-like systems.
E. Johnson et al. (1996)	Am. MCDF.
W. R. Johnson et al. (1996)	E1 transitions for Li-like (Z=3-100), Na-like (Z=11-100) systems and the alkali atoms K-Fr.
W.-Y. Liu et al. (1996)	Rydberg levels of Cs in strong magnetic field.
W. C. Martin and Sugar (1996)	ds^2p levels of Zr-Rf. Includes CI with $(d+s)^3p$.
Pak et al. (1996)	D-line of Na-like ions. Includes a phenomenological Lamb-shift model.
Quinet (1996)	Pd II.
Rakowitz and Marian (1996)	FS splitting of Tl ground state. Different radial distributions of $np_{1/2}$ and $np_{3/2}$ important.
M: S. Safronova et al. (1996a)	$n = 2$ levels of Be-like systems, Z=4-100.
M. S. Safronova et al. (1996b)	$n = 2$ levels of B-like systems, Z=5-100.
M.-L. Tan et al. (1996a)	Cu-like Ag^{50}.
M.-L. Tan et al. (1996b)	Bi^{54+}.
Thøgersen et al. (1996)	FS of Ir^- and Pt^-. MCDF.
Umemoto and Saito (1996)	Electron configurations of superheavy elements, Z=121-131. g-electrons appear at Z=126.
Vijayakumar and Gopinathan (1996)	SO splittings of TM atoms and ions. Cr ... Au. DFT/DF.
Visscher et al. (1996a)	FS splitting of the Cl atom. Effect of triples important.
W. J. Wang et al. (1996)	O-like ions, Z=52-79. MCDF.
Wijesundera et al. (1996)	FS levels of ns^2np Ca^- - Ba^-.
Ali (1997)	FS splitting of Ga-like atoms
Beck (1997a)	$3d^4$ systems Xe^{32+}, ... Gd^{42+}. J = 2,3.

Reference	Comments
Beck (1997b); Beck and Datta (1993)	FS for $(d+s)^3$ states of La I, Zr II, Hf II.
Bhatia and Drachman (1997)	Rydberg states of Li.
Biémont et al. (1997a)	Lowest $5g-6h$ supermultiplet of Fe II.
Bonnelle et al. (1997)	nd x-ray emissions (n=3-5) in U^{4+} compounds. MCDF.
M. H. Chen and Cheng (1997a)	$2s^2$ and $2s2p$ ($J=1$) states of Be-like ions, $Z=10...92$.
M. H. Chen and Cheng (1997b)	$3s^2$ and $3s3p$ states of Mg-like ions, $Z=12...42$.
Chou and Johnson (1997)	Cu-, Ag- and Au-like ions.
Dzuba and Gribakin (1997)	M^-, M=Ca-Ra.
Elander and Yarevsky (1997)	Antiprotonic helium, $\bar{p}He^+$. Relativistic and QED effects.
Ishikawa and Koc (1997)	B-In, Cu-Au.
Johnson et al. (1997b)	Mg I, Al II, Al I, Tl II, Tl I, Pb I, Bi II, Bi I.
Johnson et al. (1997c)	n=3 states of B-like Na.
Jönsson and Froese Fischer (1997b)	Mg-like $3s^2$-$3s3p$ transitions. $Z \leq 18$.
Korobov and Bakalov (1997)	Metastable states of antiprotonic He.
Rosberg and Wyart (1997)	Au II.
M. S. Safronova et al. (1997ab)	$n=3$ levels of Be-like systems, Z=4-30,54.
Sekiya et al. (1997)	$6s$ and $4f$ ionized states of Ln; Ln=Ce-Lu.
Shukla et al. (1997)	FS splitting of Pb-like systems, Pb→Po^{2+}.
Vilkas et al. (1997)	Be, Be-like Ne.
Wahlgren et al. (1997)	SO splitting of the Tl atom. BP/DK.
Yan and Drake (1997)	FS of Li $2p$ state. Includes QED.
Bhatia and Drachman (1998c)	Binding energy of Ps^-.
Biémont et al. (1998)	$s-p$ and $s-d$ transitions of Fr. Tests on Rb, Cs.
Bruch et al. (1998a)	$3lnl'$ states of Na-like Cu.
Bruch et al. (1998b)	$3lnl'$ states of Na-like Fe.
G.-X. Chen and Ong (1998a)	Fe XXIII.
Dzuba and Johnson (1998)	Ba. Test new MBPT+CI B-spline method.
Eliav et al. (1998b)	Bi, E115 (eka-Bi). DFB+CCSD.
Eliav et al. (1998c)	La, Ac, E121 (eka-Ac). Ac^{2+} and Ac^+ have $7s^1$ and $7s^2$ ground states, respectively. La^{2+} and La^+ have $5d$ and $5d^2$, respectively.
Feldmann et al. (1998)	S states of 3-electron atoms. BP Hamiltonian and explicitly correlated wave functions lead to individual divergencies which, however, cancel.
Fritzsche et al. (1998)	P-like iron-group ions, Z=22-32, $3s3p^4$ and $3s3p^23d$ configurations.
Froese Fischer et al. (1998a)	O isoelectronic series, Z=9-18. $2p^4-2p^33s-2s2p^5$ transitions.
Froese Fischer et al. (1998b)	Li isoelectronic series, Z=3-8.
Godefroid et al. (1998)	Review on atomic structure calculations.
Jönsson and Froese Fischer (1998)	$2s^2$-$2s2p\ ^3P_1$ intercombination transition in C III.
Jönsson et al. (1998)	Be isoelectronic sequence. Z=7-28,...42.
Kohstall et al. (1998)	Si-like ions, Z=16-36, $3s3p^3$, $3s^23p3d$.
Lindroth et al. (1998)	H^- resonances converging to H($n=2$) threshold.
W.-J. Liu and Dolg (1998)	$f^{n+1}d^0 \rightarrow f^nd^1$ transitions of La-Yb. Several density functionals compared.
W.-J. Liu et al. (1998c)	IPn; n=1-4, $5f-6d$ excitation energies of Ac-No. DFT and PP methods compared.

Reference	Comments
Pyykkö et al. (1998)	Estimated valence-electron Lamb shifts for Li-E119, Cu-E111. About -1% of kinetic Dirac shifts for large Z.
Qu et al. (1998a)	Li-like core-excited $1s2snp\ ^4P$ states, Z=4-8.
Qu et al. (1998b)	Li core-excited $1s2snl$ states.
Rakowitz et al. (1998)	Ir^+. A new SO operator tested.
M. S. Safronova et al. (1998)	Na-like systems, Z=11-16.
U. I. Safronova et al. (1998a)	$n = 3$ states of B-like systems, Z=6-30.
Sanoyama et al. (1998)	Low-lying levels of Ln^{3+}; Ln=Ce-Eu, Tb-Yb. Compare different PP. Semi-core correlation ($4d, 5s, 5p$) important.
Santos et al. (1998a)	$2s_{1/2} - 2p_{3/2}$ transitions of Li-like to Ne-like Bi, Th and U. Includes QED via Welton potential.
Shabaev (1998a)	QED theory of nuclear recoil in atoms to all orders in αZ.
Taïeb et al. (1998)	Signature of relativistic effects in atom-laser interactions at ultrahigh intensities.
Vilkas et al. (1998a)	B-like ions, Z=10 ... 42. MCDF.
Vilkas et al. (1998b)	O-like Fe. Low-lying states.
Yan and Drake (1998)	Relativistic and QED energies in Li $2s$, $2p$ states and in Li^+.
Yan et al. (1998)	$2s$ and $2p$ states of Li-like systems. Z=3-20 + extrapolations.
Beck (1999)	Energies of the nearly Z-independent $J = 3 \rightarrow 2$ transition of the $3d_{3/2}^3 3d_{5/2}$ systems W^{52+} and Bi^{61+}.
Bhatia and Drachman (1999)	C IV excitation energies.
Drake (1999)	High-precision theory of He.
Dzuba et al. (1999a)	Positron bound to Cu atom. Affinity 170 meV.
Dzuba et al. (1999bc)	Sensitivity of atomic data to space-time variation of natural constants.
Froese Fischer (1999)	Review on transitions in lighter atoms. BP/Dirac.
Gayasov and Joshi (1999)	$4d^9 - 4d^8 5p$ in La XIII and Ce XIV
Petit (1999)	U I. $f^3ds^2 + f^3d^2s$.
Quinet et al. (1999)	Ln II.
M. S. Safronova et al. (1999)	Alkali metals, Na-Fr.
U. I. Safronova et al. (1999c)	E1 transitions between $n = 2$ states in B-like ions. Z=6-100.
Tachiev and Froese Fischer (1999)	Be-like systems, Z=4-12. $2s2p$, $2p^2$, $2s3s$, $2s3p$, $2s3d$ excited levels. BP.
Vilkas et al. (1999)	O-like systems, Z=8-60.
Yan and Ho (1999)	Relativistic effects in positronium hydride (PsH, e^-e^+p).

Table 5.3: Auger and autoionization processes.

Reference	Comments
M. H. Chen (1993a)	Angular distributions in resonant Auger decay. Intermediate coupling.
Cornille et al. (1993)	Autoionization rates for Be-like systems.
d'État et al. (1993)	X-ray spectroscopy of highly charged ions, interacting with surfaces. A review.
Fritzsche (1993)	Xe resonant $4d^{-1}6p$ Auger spectra. Angular distribution.
Kotochigova and Lambropoulos (1993,1994)	Multiphoton ionization and autoionization of Si I.
Lohmann (1993)	Correlation effects on Hg Auger spectra. MCDF.
Mäntykenttä (1993)	Channel interaction and relaxation effects in Xe $N_{4,5}OO$ Auger transitions.
Mäntykenttä et al. (1993)	Electron correlation in $4d$ hole states of Ba studied by Auger and photoelectron spectroscopy.

Reference	Comments
Pindzola (1993)	Parity-violation effects on Auger-electron emission from highly charged atomic ions. $2s^2\ J = 0$ of U^{90+}.
Tulkki et al. (1993a)	Auger decay of $2p_{3/2}^{-1}ns$ resonances in Ar.
Tulkki et al. (1993b)	Effect of channel interaction, exchange and relaxation on the angular distribution and spin polarization of Auger electrons from noble-gas atoms.
Tulkki and Mäntykenttä (1993)	Subshell-dependent relaxation in the Auger effect.
M. H. Chen and Reed (1994)	Angular Distribution of Auger electrons after electron-impact ionization. Be-like ions, Z=12...42.
Flambaum et al. (1994)	Chaotic spectrum of Ce.
Hsu et al. (1994)	^4P series of Li. Autoionization.
Ivanov and Safronova (1994)	Correlation and relativistic effects for $3l3l'$ autoionization states.
Kivimäki et al. (1994)	Kr and Xe satellite Auger spectra.
Lohmann and Fritzsche (1994)	KLL Auger spectra of alkali atoms.
M. S. Safronova et al. (1994)	Autoionization states of Be-like ions. Z-dependence.
U. I. Safronova and Nilsen (1994)	Autoionization states of Li-like ions with large n.
Tulkki et al. (1994)	Effect of initial-state–final-state CI on anisotropy of resonant Auger decay of Kr $3d^{-1}5p$ and Xe $4d^{-1}6p$ states.
Aksela et al. (1995)	Resonant Auger decay of Xe $4d_{3/2,5/2}^{-1}6p$.
Cole et al. (1995)	Auger parameter shifts from free atoms to solids, in alkali and alkaline earth metals.
U. I. Safronova et al. (1995)	Radiative and autoionization TP for $1s2l''nl - 1s^2n'l'$; $n, n' = 2, 3$ transitions for He-like ions.
Aksela et al. (1996a)	Review on resonant and nonresonant Auger recombination.
Aksela et al. (1996b)	Resonantly excited $3d_{3/2,5/2}^{-1}5p$ states of Kr.
Aksela et al. (1996c)	Resonantly excited $4d_{3/2,5/2}^{-1}6p$ states of Xe.
Aksela and Mursu (1996)	Resonant $2p^{-1}4s$ and $3p^44s$ states of Ar.
Flambaum et al. (1996)	'Narrow chaotic compound autoionizing states in atomic spectra. Simultaneous excitation of several electrons $\Rightarrow$ dense spectrum $\Rightarrow$ chaos. Ce.
Gel'mukhanov et al. (1996)	Auger spectra for molecular-field-split core levels. H_2S.
M. H. Chen et al. (1997)	K-shell Auger and radiative transitions for C-like systems, $6 \leq Z \leq 54$.
U. I. Safronova et al. (1997)	Autoionizing states of Li-like ions with high n.
M. Cohen et al. (1998)	Excitation autoionization rate from ground and excited levels. Li-like to S-like Ar.
Indelicato et al. (1998)	K-, L-, and M-shell IP for elements with Z=10-100. 'Auger shifts' included.
Qu et al. (1998a)	Li-like core-excited $1s2snp\ ^4P$ states, Z=4-8.
Qu et al. (1998b)	Li core-excited $1s2snl$ states. Autoionization.
U. I. Safronova and Johnson (1998)	Autoionizing rates for doubly excited $2lnl'$ states of He-like ions.
U. I. Safronova et al. (1998b)	Autoionization rates for $1s^{-1}2p^2$, $1s^{-1}2s^{-1}2p^3$ and $1s2p^4$ states of B-like ions, $Z = 6 - 54$.
Cornille and Dubau (1999)	Autoionization of $1s2s^22p^2$, $1s2s2p^3$ and $1s2p^4$ states of B-like ions, Z=6-54.
Safronova and Shlyaptseva (1999)	Autoionization rates and energies for C-, N-, O-, and F-like ions with $Z = 6 - 54$.

Reference	Comments
Santos et al. (1999)	Radiative and non-radiative decay rates of $2s$ (L_1) hole states in Yb and Hg. MCDF and MBPT.
L.-R. Wang et al. (1999)	Doubly excited states in photoionization of Zn. Autoionization resonances.

Table 5.4: Ionization potentials and electron affinities.

Reference	Comments
Arnau et al. (1992)	EA of Group-13 atoms, Al-Tl.
Chakravorty et al. (1993)	IP for 3-18 electrons, Z=3-36, .. Includes Dirac-Breit +QED.
K. T. Chung et al. (1993)	IP of Be-like systems, Z=4-10,15,20.
Datta and Beck (1993)	Possible EA(Ln) with $4f$-electron attachment. Negative results for the nf^{14} Tm^- and Md^-.
Fricke et al. (1993)	IPn of Ta, E105 (Db). MCDF.
Hughes and Kaldor (1993)	EA of F-At. Fock-space CC method.
Ilyabaev and Kaldor (1993)	Relativistic coupled-cluster approach for open-shell atoms. IP of Li, C, O, F, Na.
Vosko and Chevary (1993)	Electron shell filling of Ln anions: Lu^- is $5d^16s^26p^1$.
Woon and Dunning (1993)	EA of Al-Cl. Includes SO.
Datta and Beck (1994)	Th^- can have both $6d^27s^27p$ and $6d^37s^2$ bound states. EA 0.365 and 0.189 eV, respectively.
Dinov et al. (1994)	EA of Ce. $6p$ or $5d$ attachment.
Dzuba and Gribakin (1994)	Correlation-potential method for negative ions.
Eliav et al. (1994a)	IP and EA of Au. DFB+CCSD.
Eliav et al. (1994c)	IP and EA of alkali metals, Li-Fr. DFB+CCSD. Average IP error 0.09%, EA error 4-9%.
Eliav et al. (1994e)	IP and EA of E111 (eka-Au).
Mitas (1994)	PP QMC calculation of IP and EA of Fe.
Sundholm and Olsen (1994)	EA of Ca. PT relativity.
Dinov and Beck (1995a)	EA of $6p$ electrons in Pr.
Dinov and Beck (1995b)	EA for U. $7p$ attachment.
Eliav et al. (1995a)	EA of Rf (E104) 6.01 eV. DFB+CCSD.
Eliav et al. (1995c)	IP and EA for Yb, Lu, Lr.
Eliav et al. (1995d)	IP of eka-mercury, E112.
García de la Vega (1995)	Relativistic corrections to EA of Li-I. Mostly BP without SO.
Liaw (1995)	Bound states of Ca^-. No EA in Brueckner approximation.
Sundholm (1995)	EA of Sr and Ba. PT relativity.
Tatewaki et al. (1995)	$6s$ and $4f$ IP Cs, Ba, La-Lu. DF.
Yan and Drake (1995)	IP of Li.
J.-M. Yuan (1995)	Without relativity, $d_{3/2}$ state of Ba^- would be bound.
Dinov and Beck (1996)	EA for Pa. $7p$ attachment.
Eliav et al. (1996a)	IP of Ba, Ra.
Eliav et al. (1996b)	EA of E118. The first rare gas with an EA. Both relativity and correlation essential.
Eliav et al. (1996c)	IPn; n=1-4 and EA of Tl, E113 (eka-Tl).
Glushkov et al. (1996)	EA of Ca and Sr.
Salomonson et al. (1996)	EA of Ca and Sr.
Thøgersen et al. (1996)	FS of Ir^- and Pt^-. MCDF.
Wijesundera et al. (1996)	FS levels of ns^2np Ca^- - Ba^-.
Andersen et al. (1997)	Negative alkaline-earth ions.

Reference	Comments
Avgoustoglou and Beck (1997)	EA of Ca-Ba, Yb.
Dzuba and Gribakin (1997)	FS of EA of Ca-Ra.
Eliav et al. (1997)	EA of B-Tl.
Forstreuter et al. (1997)	IPn of Ln, Ln=Ce→Lu. DFT tested.
Ishikawa and Koc (1997a)	IP of B-In, Cu-Au.
Ishikawa and Koc (1997b)	IP of Zn, Cd.
Jursic (1997)	EA for several metal atoms from DFT and HF-MP4, QCISD.
King (1997,1999)	High-precision calculations on the Li atom. Review.
Koga et al. (1997)	IP and EA for $Z \leq 54$. Relativistic and mass corrections included. PT.
Miadoková et al. (1997)	Standardized basis sets for highly correlated DK calculations of electric properties. IP of Li-Fr, Be-Ba.
Neogrády et al. (1997)	IP and EA of Cu-Au. R/NR. SR DK CCSD(T).
Sekiya et al. (1997)	$6s$ and $4f$ ionized states of Ln; Ln=Ce-Lu.
Z. W. Wang and Ge (1997)	IP of Li-like Sc-Zn.
Wijesundera (1997)	EA of B-Tl. MCDF.
Dzuba and Gribakin (1998)	Yb^- $6p_{1/2}$ is a resonance at 0.02 eV and not a bound state.
Eliav et al. (1998b)	IP and EA of Bi, E115 (eka-Bi).
Eliav et al. (1998c)	IP and EA of La, Ac, E121 (eka-Ac).
Glushkov et al. (1998)	EA of Si-Pb.
Indelicato et al. (1998)	K-, L-, and M-shell IP for elements with Z=10-100. The $1s$ Lamb shift of heavy elements.
W.-J. Liu and Dolg (1998)	IPn of La-Yb; n=1-4. Several density functionals compared.
W.-J. Liu et al. (1998c)	IPn; n=1-4, $5f - 6d$ excitation energies of Ac-No. DFT and PP methods compared.
O'Malley and Beck (1998)	EA of Sn.
Wijesundera and Parpia (1998)	EA of C, N, P.
Pyykkö et al. (1998)	Lamb shifts of ns valence electrons of neutral Li-E119, Cu-E111 estimated.
Vilkas et al. (1998b)	IP of Zn.
Yan and Drake (1998)	Relativistic and QED contributions to IP of Li.
Biémont et al. (1999)	IP for Li–Sn.
Chaudhuri et al. (1999a)	IP of Li-Fr, B-Tl.
Chaudhuri et al. (1999b)	IP of Li, Na, Be, Mg.
G.-X. Chen and Ong (1999b)	EA of B-Tl, C-Pb.
de Oliveira et al. (1999)	EA of H, B-F, Al-Cl. PT relativity.
Dzuba et al. (1999)	Cu. EA 1.218 eV (exp. 1.236 eV), positron affinity 0.170 eV.
Godefroid and Froese Fischer (1999)	Isotope shift in oxygen EA. FS of the anion.
Iliaš and Neogrády (1999)	IP of Zn-Hg.
Johnson et al. (1999)	IPn; n=1-6 of Cr-Sg(E106).
Labzowsky et al. (1999b)	Lamb shifts of ns valence electrons of neutral Li-E119, Cu-E111, Hg^+, Tl^{2+} calculated.
Lim et al. (1999)	IP of the alkali atoms Li-E119. CCSD(T).
J. M. L. Martin and de Oliveira (1999)	EA of H-Cl (Z=1-17). Very precise. PT.
Norquist et al. (1999)	EA of Ru.
O'Malley and Beck (1999)	EA of La. $6p$ or $5d$ attachment.

Reference	Comments
M. S. Safronova et al. (1999)	IP of Na-Fr.
Sundholm et al. (1999)	EA of Ga and In, 0.297(13) and 0.374(15) eV, respectively.

Table 5.5: Supercritical ($Z > 137$) systems.

Reference	Comments
Momberger et al. (1991, 1993)	Electron-positron pair production in collision of two naked nuclei. U+U.
Rumrich et al. (1991,1993)	Pair creation in relativistic heavy-ion collisions.
Ionescu et al. (1993)	Collective excitations of the QED vacuum.
Maier et al. (1993)	Time-dependent 1D Dirac square well: Pair production.
Müller-Nehler and Soff (1994)	Electron excitations in superheavy quasimolecules.
J. Thiel et al. (1994,1995)	Electron-positron pair creation in relativistic heavy-ion collisions.
Eichler (1995)	Charge transfer from the negative-energy continuum. Alternative pair-production mechanism.
Eichler and Belkacem (1996)	Gauge transformations for coupled-channel calculations of pair production.
Ionescu and Eichler (1996)	Pair creation in heavy-ion collisions as a charge-transfer process.
Alscher et al. (1997)	Electron-positron pair production in heavy-ion collisions.
V. I. Matveev et al. (1997)	LCAO solution of two-centre Dirac equation. Supercritical limit obtained.
Olsen and Kunashenko (1997)	Channeling of relativistic electrons in crystals. Electron-positron production. Dirac equation in cylindrical coordinates.
Dietz and Pröbsting (1998)	Electron-positron production in intensive laser fields.
Segev and Wells (1998)	Pair production in ultrarelativistic heavy-ion collisions.
Busic et al. (1999)	Electron-positron production with electron capture. U^{92+}-U^{92+}
Ionescu and Belkacem (1999)	Relativistic collisions of highly-charged ions. Time evolution of QED vacuum solved numerically.
Matrasulov et al. (1999)	Dirac electron in the field of two opposite charges. $Z < 137$ and $Z > 137$ considered.

Table 5.6: Electromagnetic transition probabilities.

Reference	Comments
Liaw (1992b)	E1 oscillator strengths for alkali-like ions.
Y. Zhang et al. (1992b)	Na-like Nb.
Baluja et al. (1993)	Allowed transitions in Fe XXI.
Beideck et al. (1993)	Au II $5d^9 6p$ lifetimes.
Bugacov and Shakeshaft (1993)	Multiphoton transitions in strong fields. Inclusion of photon momentum $\Leftrightarrow$ no dipole approximation. H^- photodetachment.
S. Cheng et al. (1993)	Branching ratio for M1 decay of $2s$ H-like Kr.
X.-L. Cheng et al. (1993)	Ni-like ions, $47 \leq Z \leq 54$.
Chung (1993)	Theory of transition rates of few-electron ions.
Curtis (1993)	$nsnp$ states of Cd- and Hg-like systems.
Harra et al. (1993)	He-like Ni. $1s2l$, $1s3l$. MCDF. E1,2 and M1,2 TP.
Judd (1993a)	Spin-dependent E1 radiation.
Judd (1993b)	Two-photon absorption in Ln compounds.

Reference	Comments
Kwato Njock et al. (1993)	E1 radial integrals in semiclassical Coulomb approximation.
La John and Luke (1993)	Spin-forbidden transitions in P II.
Lavin and Martin (1993)	B isoelectronic sequence.
Lavin et al. (1993)	Singlet-singlet transitions for Zn- and Cd-like systems.
Liaw (1993a)	Cs.
Liaw (1993b)	Alkali metal atoms in the Brueckner approximation.
Marcinek and Migdalek (1993a)	Al I isoelectronic series.
Marcinek and Migdalek (1993b)	Ga I isoelectronic series.
Marketos and Zambetaki (1993)	Two-photon non-resonant transitions on O III.
Marketos et al. (1993)	O III TP.
Migdalek and Stanek (1993)	$5s^2 - 5s5p$ transitions in the Sr sequence.
Papp et al. (1993)	L-x-ray intensity ratios. DF/DS/experiment.
Radozycki and Faisal (1993)	Multiphoton ionization of strongly bound relativistic electrons in very intense laser fields.
Tiwary (1993); Tiwary and Kandpal (1994)	R/NR oscillator strengths in Na sequence.
Q.-S. Wang and Stedman (1993)	Derives from FW an E1 term of form $q\mathbf{s} \cdot \dot{\mathbf{A}} \times \mathbf{p}/2m^2c^2$. Applications to lanthanides.
Aashamar and Luke (1994a)	Sextet levels of Cr II.
Aashamar and Luke (1994b)	The $4p\ ^{6,4}P^o_J$ and $4p\ ^6D^o_J$ levels of Cr II.
Biémont et al. (1994)	TP for the Ga $4s^24p$ isoelectronic sequence.
Biémont et al. (1994c)	$4s - 4p$ transitions in neutral P.
S. Cheng et al. (1994)	M1 decay of $1s2s\ ^3S$ He-like Kr.
W.-Y. Cheng and Huang (1994b)	Z-dependence of oscillator strengths for Be-like ions.
X.-L. Cheng et al. (1994)	Ni-like ions, $72 \leq Z \leq 79$.
Cornille et al. (1994)	Radiative data for Ne-like ions.
Gębarowski et al. (1994)	$3s^23p - 3s^23d$ transitions for Al-like sequence.
Kwato Njock et al. (1994b)	Oscillator strengths of Li-like ions from exact QDT.
Land et al. (1994)	Selection rules for dipole radiation from a relativistic bound state.
Lavin et al. (1994)	FS transitions in Cu isoelectronic sequence, $Z \leq 92$.
Lavin and Martin (1994)	Triplet-triplet transitions in Cd-like ions.
Marinescu et al. (1994b)	Two-photon excitation of Rb, $5\ ^2D$.
Marketos (1994)	E2 transitions between even O III levels.
P. Martin et al. (1994)	Triplet-triplet transitions in Zn-like ions. QDT.
Padma and Deshmukh (1994)	Oscillator strengths for $2p$ ionization near threshold.
Parente et al. (1994)	M1 and E2 hyperfine quenching of Ti-like ions, $3d^4$, J=4, Z=55-92.
Schneider et al. (1994b)	M1 hfs-level lifetime in H-like $^{209}Bi^{82+}$.
Tong et al. (1994a)	Relativistic effect on atomic radiative processes. A 'zero' of the H-like E1 transition matrix element found.
Tong et al. (1994b)	TP for O III.
Vilkas et al. (1994)	E1 TP for O-like sequence.
H. L. Zhang and Sampson (1994a)	Oscillator strengths for B-like ions, Z=8-92. $\Delta n = 0, n = 2$.
H. L. Zhang and Sampson (1994b)	Oscillator strengths for B-like ions, Z=8-92. $n = 2$ - $n = 3$.
Aboussaïd et al. (1995)	Hyperfine-induced transitions in He-like ions. $1s2p\ ^3P_0$, Z = 9, 11, 13.
Beck and Datta (1995)	Nb II $4d^35p$ [$^5G_3$ and $^3D_3$] $\rightarrow (4d + 5p)^4$ TP.
Dzuba et al. (1995)	Fr.

Reference	Comments
Fritzsche et al. (1995)	Cl-like ions, $3p^4 3d$ configurations.
Mendoza et al. (1995)	Al I sequence.
Nana Engo et al. (1995)	Relativistic semiclassical dipole matrix elements for $nlj \rightarrow n'l'j'$ transitions in non-hydrogenic ions.
Mårtensson-Pendrill (1995)	Tl I $7s \rightarrow 6p$ E1, $6p_{3/2} \rightarrow 6p_{1/2}$ E2 TP.
U. I. Safronova et al. (1995)	Radiative and autoionization TP for $1s2l''nl - 1s^2n'l'$; $n, n' = 2, 3$ transitions for He-like ions.
Uylings and Raassen (1995)	Accurate calculation of TP using orthogonal operators. Include valence correlation in transition matrix. $5d^9 \rightarrow 5d^8 6p$ in Hg IV ... Bi VII.
Ynnerman and Froese Fischer (1995)	Be-like systems, Z=6...42. The E1 $2s^2\ ^1S_0 - 2s2p\ ^1P_1$ and the forbidden $2s^2\ ^1S_0 - 2s2p\ ^3P_1$ energies and TP.
Bharadvaja and Baluja (1996)	E1 TP in Li, F, Na and Cu isoelectronic series. Parametric fit.
Brage et al. (1996); Brage et al. (1999)	Tl II, Tl III.
Fleming et al. (1996)	Resonance line of Be sequence.
Indelicato (1996)	Correlation and negative continuum effects for the M1 transition in two-electron ions. MCDF.
Johnson et al. (1996)	E1 TP for Li-like (Z=3-100), Na-like (Z=11-100) systems and the alkali atoms K-Fr.
Luke (1996)	Quartet multiplets in V I.
Quinet (1996)	Pd II.
W. J. Wang et al. (1996)	O-like ions, Z=52-79. MCDF.
Ali (1997)	M1 and E2 transitions of Ga-like systems.
Biémont (1997a,1997b)	E1, E2, E3; M1, M2, M3 TP for Ni-like and Pd-like systems.
Biémont et al. (1997b)	$4d^9 5p$ levels of Ag II.
M. H. Chen et al. (1997)	K-shell Auger and radiative transitions for C-like systems $6 \leq Z \leq 54$.
M.-K. Chen (1997)	E1 TP for He-like ions, Z=3...10.
Chou and Johnson (1997)	Cu-, Ag- and Au-like ions.
Curtis et al (1997)	Methods for intermediate-coupling amplitudes. $2s^2 - 2s2p$ transitions in Be-like, $6s^2 6p^2 - 6s^2 6p7s$ in Pb-like systems.
Henderson et al. (1997)	Au-like systems, Z=79-83.
Indelicato (1997)	E2 and two-electron one-photon E1 transitions of $2s3p$ $^3P_0$ states of Be-like ions. MCDF.
Johnson et al. (1997a)	M1 hfs of 2 ^3P levels of He-like ions, Z=2-51. Hfs-induced quenching of the levels.
Jönsson and Froese Fischer (1997b)	E1,E2 and M1,M2 TP for Mg-like $3s^2$-$3s3p$ transitions.
Kotochigova et al. (1997)	Giant resonance in the $4d - 4f$ spectrum of Gd^{3+}, $4d^9 4f^8$. MCDF.
Kovalik (1997)	Effects of relativity on the KL_1L_2 ($^3P_0$) transition rate of $^{159}_{65}$Tb.
Lavin et al. (1997)	FS transition in Al isoelectronic sequence.
Marketos and Nandi (1997)	O II levels.
Nana Engo et al. (1997)	Supersymmetry-inspired R and QR quantum-defect theory. Applications on transition matrix elements.
Porsev (1997)	E1 lifetimes of low-lying odd-parity levels of Sm.
Quinet (1997)	Cr II.
Sampson and Zhang (1997)	Collision strengths for hfs transitions.

Reference	Comments
Skripnikova and Zapriagaev (1997)	Correlation and relativistic corrections to TP in He-like ions.
Szymanowski et al. (1997)	Two-photon bound-bound amplitudes in H-like atoms.
Velasco et al. (1997)	Neutral F.
H. L. Zhang and Sampson (1997)	Oscillator strengths for $(n = 2) - (n = 3)$ transitions in C-like ions, Z=9-54.
Avgoustoglou and Beck (1998)	$np^6 \rightarrow np^5(n+1)s$ E1 resonance lines of Ne–Xe.
Beck (1998)	Cs II $5p^5\ 6p$ level lifetimes.
Biémont et al. (1998)	$s - p$ and $s - d$ TP of Fr.
Derevianko et al. (1998)	Negative-energy contributions to En and Mn TP in He-like ions. Significant for M1 $3\ ^3S_1 \rightarrow 2\ ^3S_1$.
Fritzsche et al. (1998)	P-like iron-group ions, Z=22-32, $3s3p^4$ and $3s3p^23d$ configurations.
Froese Fischer and Rubin (1998)	E2 and M1 TP for Fe IV.
Froese Fischer et al. (1998a)	O isoelectronic series, Z=9-18. $2p^4 - 2p^33s - 2s2p^5$ transitions.
Froese Fischer et al. (1998b)	Li isoelectronic series, Z=3-8.
He et al. (1999)	FS transition of Br. M1.
Jönsson and Froese Fischer (1998)	$2s^2$-$2s2p\ ^3P_1$ intercombination transition in C III.
Jönsson et al. (1998)	Be isoelectronic sequence. Z=7-28,...42.
Y.-K. Kim et al. (1998)	Failure of MCDF at NR limit. The wave function for specific J may not reduce to the LS limit. Be-like example. Effects on TP discussed.
Kohstall et al. (1998)	Si-like ions, Z=16-36, $3s3p^3$, $3s^23p3d$.
Lagmago Kamta et al. (1998)	Semiclassical KG dipole matrix elements.
Marinescu et al. (1998)	Radiative transitions of Fr.
Maul et al. (1998)	'Stark quenching' in laser fields for PNC observations. One- and two-photon transitions of Be-like $2s2p\ ^3P_0$ levels.
O'Malley and Beck (1998)	M1 decay rates of Sn^-, $5p^3$.
Pal'chikov (1998)	En and Mn TP of arbitrary n for H-like atoms. Z=1-92.
Prosser (1998)	Energy spectrum of H atom in photon field. Line broadening.
Romero and Aucar (1998, 1999)	Relativistic corrections to generalized oscillator strength sum rules.
M. S. Safronova et al. (1998)	Na-like systems, Z=11-16.
Schmitz et al. (1998)	3D relativistic calculations of strong-field photoionization. Phase-space averaging, classical method.
Shabaev (1998b)	TP between M1 hfs levels of H-like ions related to the bound-electron g-factor.
Shi et al. (1998ab)	$4p - 5s$ excitations of Kr.
Siegel et al. (1998)	E1 TP for the Na sequence, Na I - Ca X.
Yan et al. (1998)	$2p - 2s$ TP of Li-like systems. Z=3-20 + extrapolations.
Beck (1999)	$M1$ decay rate of the nearly Z-independent $J = 3 \rightarrow 2$ transition of the $3d^3_{3/2}3d_{5/2}$ systems W^{52+} and Bi^{61+}.
J. Chen et al. (1999)	High-order harmonics for H-like atom in ultrastrong laser field.
Donnelly et al. (1999)	Oscillator strengths of Cu^+.
Froese Fischer (1999)	Review on transitions in lighter atoms. BP/Dirac.
Henderson et al. (1999)	$5d^96p$ levels in Hg III.
Horodecki et al. (1999)	Forbidden lines in Pb I, $6s^26p^2$. MCDF.
Kohstall et al. (1999)	Cl-like ions, $3s3p^6$, $^2S_{1/2}$.

Reference	Comments
Z.-S. Li et al. (1999)	21 levels of Ge I. $4p4d$, $4p5d$, $4p6s$.
Merkelis et al. (1999)	M1 and E2 transitions in in the N I sequence.
Nahar (1999)	E1 FS transitions of Si-like Fe XIII. 307 683 transitions.
Norquist et al. (1999)	M1 decay of Ru^-, $d^7s^2\ ^4F$.
O'Malley and Beck (1999)	E1 TP of La^-. $6p$ or $5d$ attachment.
Ozdemir and Karal (1999)	Oscillator-strengths from relativistically corrected HF.
Porsev et al. (1999b)	Low-lying levels of Yb.
Pradhan (1999)	TP for Fe V, XXIV, XXV. BP R-matrix method.
Quinet et al. (1999)	Ln II.
M. S. Safronova et al. (1999)	Alkali metals, Na-Fr.
U. I. Safronova et al. (1999a)	Be-like ions. $2l_12l_2 - 2l_33l_4$ TP. Z=6-100.
U. I. Safronova et al. (1999b)	M1 transitions in Be-like ions, Z=4-100. Importance of negative-energy states discussed.
U. I. Safronova et al. (1999c)	E1 transitions between $n = 2$ states in B-like ions. Z=6-100.
U. I. Safronova et al. (1999d)	$2l_12l_2 - 2l_32l_4$ lines in Be-like ions. $Z = 4 - 100$.
Santos et al. (1999)	Radiative and non-radiative decay rates of $2s$ (L_1) hole states in Yb and Hg. MCDF and MBPT.
Santos et al. (1998b)	Two-photon decay rates of $2s$-level in H-like ions. Z=1-100.
Tachiev and Froese	Be-like systems, Z=4-12. $2s2p$, $2p^2$, $2s3s$,
Fischer (1999)	$2s3p$, $2s3d$ excited level lifetimes. BP.
Yan and Ho (1999)	Relativistic effects in positronium hydride (PsH, e^-e^+p). Two-photon annihilation rate calculated.
H. L. Zhang and Sampson (1999)	Oscillator strengths for the 105 Δn=0 transitions with $n = 2$ in the N-like ions, Z=12-92.

Table 5.7: Polarizabilities, dispersion and screening constants.

Reference	Comments
Feiock and Johnson (1968)	Magnetic shielding factors. Use Dirac current!
Bondarev and Kuten (1993)	Polarizability tensors for H-like $ns_{1/2}$ and $np_{1/2}$ states. Due to M1 hfs.
Fuentealba and Reyes (1993)	Polarizabilities and hyperpolarizabilities of Li-Cs.
Kellö et al. (1993)	Polarizabilities of K-Fr. PT relativity.
Le et al. (1994)	DC Green function. Polarizability of H-like atoms.
Schwerdtfeger et al. (1994b)	Polarizability of Hg.
van Wijngaarden and Li (1994)	Polarizabilities of Cs s, p, d, f states.
Z.-W. Wang and Chung (1994)	Dipole polarizabilities of Li-like systems, Z=3-50.
Baluja (1995)	Dipole polarizability of H-like ions.
Kellö and Sadlej (1995a)	Polarizabilities of M^{q+}; M=Zn-Hg; q=0-2.
Nicklass et al. (1995)	Dipole and quadrupole polarizabilities of Ne-Xe.
Szmytkowski and Alhasan (1995)	Polarizabilities for alkaline-earth-like systems.
Hättig and Hess (1996)	Dynamic multipole polarizabilities, dispersion coefficients for Ar-Rn. SR DK.
Johnson and Cheng (1996)	Polarizabilities of He-like ions. MCDF. R/NR.
Kellö and Sadlej (1996a)	DK CCSD(T) polarizabilities of Cu-Au, Zn-Hg and their cations.
Kellö et al. (1996b)	Polarizabilities of M^-; M=Cu-Au. R/NR. DK/PT.
Neogrády et al. (1996,1997)	QR CCSD(T) polarizabilities for M,M^+; M=Cu-Au.

Reference	Comments
Dzuba et al. (1997a)	Dipole polarizability of Cs.
Henderson et al. (1997)	Exp. contributions to dipole polarizabilities of Au I - Bi V.
Miadoková et al. (1997)	Standardized basis sets for highly correlated DK calculations of electric properties. Polarizability of K-Fr, Li^+-Fr^+, Ca-Ba.
Szmytkowski (1997)	DC Sturmians and the DC Green function. Relativistic polarizability of the H-like atom, Z=1-137.
Visscher et al. (1997)	$\alpha(\omega)$ of Hg. RRPA.
Hättig and Hess (1998)	Dynamic multipole polarizabilities, dispersion coefficients for F^- to I^-. SR DK.
Coutinho et al. (1999)	Two definitions for electric polarizability, with or without the vacuum background.
Derevianko et al. (1999a)	Dipole polarizabilities and dispersion constants. Na-Fr.
Iliaš and Neogrády (1999)	Dipole polarizability of M^+; M=Zn-Hg.
Lim et al. (1999)	Polarizabilities of alkali metals Li-E119. For Fr and E119, substantial SO effects and small total values. CCSD(T).
Porsev et al. (1999b)	Electric polarizabilities for low-lying levels of Yb.
M. S. Safronova et al. (1999)	Electric polarizabilities of Na-Fr.

Table 5.8: Electric and magnetic hyperfine properties.

Reference	Comments
Acker et al. (1966)	M1 and E2 hfs for muonic atoms. Fermi nuclear potential.
Moss and Sadler (1986)	Electric quadrupole moments of one-electron atoms. In $j = \frac{1}{2}$ states due to hfs. Resolves earlier inconsistencies.
M.-K. Chen (1993)	M1 hfs of the muonic ^{3}He.
Dembczyński et al. (1993)	Co $(3d+4s)^9$ M1, E2 hfs. $Q(^{59}\mathrm{Co})$ 410(10) mb.
Dougherty et al. (1993)	M1 hfs of Cu-Au. Core polarization analyzed.
Finkbeiner et al. (1993)	M1 hfs energy and lifetime for Bi^{82+}.
Jönsson (1993)	MCDF approach to atomic hfs. B-Tl. Li-like F.
Jönsson and Froese Fischer (1993)	M1 and E2 hfs of low-lying states in Be, B, C.
Kronfeldt et al. (1993a)	Isotope shifts of Re I.
Kronfeldt et al. (1993b)	Fine and hyperfine structure of Er I, $4f^{11}5d6s6p$.
Marques et al. (1993a)	Hyperfine quenching of Be-like $1s^22s2p\ ^3P_0$.
Marques et al. (1993b)	Hyperfine quenching of Mg-like $3s3p\ ^3P_0$.
Schneider et al. (1993b)	M1 hfs of $^{209}Bi^{82+}$.
Shabaeva (1993)	Ground-state M1 hfs of Li-like Bi.
Young et al. (1993)	M1 and E2 hfs in Zr II.
G. X. Chen (1994)	Sc II, $3d^2$. Core-polarization effects.
Dzuba et al. (1994)	M1 and E2 hfs in Dy.
Mårtensson-Pendrill et al. (1994)	Yb^+ hfs, isotope shifts.
Parente et al. (1994)	M1 and E2 hyperfine quenching of Ti-like ions, $3d^4$, J=4, Z=55-92.
Schneider et al. (1994b)	M1 hfs-level lifetime in H-like $^{209}Bi^{82+}$.
Scofield and Nilsen (1994)	M1 hfs for $2p^{-1}3p$ and $2p^{-1}3s$ levels of Ne-like systems, Z=17-59.
Shabaev (1994a)	M1 and E2 hfs of H-like ions. Finite-nucleus corrections.
Yakhontov and Amusia (1994)	M1 hfs in the $1s_{1/2}{}^{(e)}\ 2s_{1/2}{}^{(\mu)}$ state of the exotic $(^4He^{2+}\text{-}\mu^-e^-)^0$ and $(^3He^{2+}\text{-}\mu^-e^-)^0$ atoms.
Aboussaïd et al. (1995)	M1 and E2 hyperfine-induced transitions in He-like ions.

Reference	Comments
	$1s2p\ ^3P_0$, Z = 9, 11, 13.
Datta and Beck (1995)	M1, E2 hfs of ^{139}La II, $(5d+6s)^2$, J=2.
Dinov and Beck (1995b)	M1, E2 hfs of U and U^-.
Fedorov et al. (1995)	M1 and E2 hfs for the (K and L) inner shells, Z=10-100. DF.
Jönsson (1995)	Large-scale MCDF calculations. Thesis.
Kroger and Kroger (1995)	Program for angular coefficients of relativistic one-electron hfs parameters.
Labzowsky et al. (1995)	Introduce the 'dynamic proton model' for hfs of H-like ^{209}Bi. Interaction between valence electron and valence proton at QED level.
Loginov (1995)	CI effects on atomic hfs at semiempirical level. Examples Sc II and Y II.
Mårtensson-Pendrill (1995)	Magnetic moment distributions in ^{203,205}Tl.
Pilkuhn (1995)	An M1 hyperfine operator between two Dirac particles, both having anomalous magnetic moments.
Shabaev et al. (1995, 1997a,1998d)	Hfs of H-like and Li-like ions.
Shabaeva and Shabaev (1995)	Interelectronic contribution to hfs of Li-like ions. $1/Z$ expansion, including QED effects. Z=5-100.
H. Y. Yang and Chung (1995)	Be-like systems, $Z = 3-10$, core-excited $1s2s2p^2(^2P)$ and $1s2p^3(^5S)$ states.
Young et al. (1995)	M1 and E2 hfs in Nb II.
X. Yuan et al. (1995a)	M1 hfs of $7p$ states of Ra^+.
X. Yuan et al. (1995b)	M1 hfs of Ca^+ and Sr^+. Results compared with trends in Groups 1, 2, 11.
Bieroń et al. (1996a)	M1, E2 hfs of $2s$ and $2p$ states of Li.
Bieroń et al. (1996b)	M1, E2 hfs of nd^2 levels of Sc^+, Y^+.
Bigeleisen (1996)	Nuclear size and shape effects in chemical reactions. Uranium redox reactions as example.
Brage et al. (1996); Brage et al. (1999)	M1 hfs in Tl II, Tl III. Large MCDF.
Crespo Lopez Urrutia et al. (1996)	Observe F=3-4 transition of H-like $^{165}Ho^{65+}$. Result deviates from tabulated magnetic moment.
Dinov and Beck (1996)	M1, E2 hfs for Pa^-.
Jönsson et al. (1996)	HFS92: A program for atomic hfs calculations. MCDF.
O'Malley and Beck (1996)	M1 and E2 hfs of Cs II and Ba III $(5d+6s+6p)$ levels.
Yan et al. (1996)	FC term of M1 hfs in Li $2s, 2p, 3s$, Be^+ $2s$. Includes QED.
Beck (1997b); Beck and Datta (1993)	M1 and E2 hfs for $(d+s)^3$ states of La I, Zr II, Hf II.
Bieroń et al (1997)	E2 hfs of $3d^2$ and $3d4p$ levels of Sc. $Q(^{45}Sc)$ -231(4) mb.
Childs (1997)	Matrix elements of hfs operators in SL and jj representations for s^N, p^N and d^N configurations.
Friar et al. (1997)	Nuclear sizes and isotope shifts. The nuclear physics perspective.
Friar and Payne (1997a)	Higher-order nuclear-polarizability corrections for hydrogen (H or D).
Friar and Payne (1997b)	Higher-order nuclear-size corrections for hydrogen.
Johnson et al. (1997a)	M1 hfs of 2 ^3P levels of He-like ions, Z=2-51. Hfs-induced quenching of the levels.
Jönsson and Froese Fischer (1997a)	SMS92: a program for relativistic isotope shift calculations.

Reference	Comments
King (1997,1999)	High-precision calculations on the Li atom. Review.
Labzowsky et al. (1997ac)	M1,E2,M3 hfs of the $2p_{3/2}$ state of H-, Li-, B- and N-like $^{209}_{83}$Bi. Interaction between valence electron and valence proton treated at QED level.
Owusu et al. (1997a)	M1 hfs in excited S states of K, Fr.
Owusu et al. (1997b)	M1 hfs in K-like system (K-Sc^{2+}) ground states.
J. R. Persson (1997)	Hfs of Yb^+.
Sampson and Zhang (1997)	Collision strengths for hfs transitions.
Shabaev et al. (1997b)	Ground-state M1 hfs splitting of H-like ions. Z=49-83.
Tulub et al. (1997)	Simulate the QED effects in many-electron atoms by a renormalized nucleus (right radius, changed charge inside). Application on M1 hfs of H-like Bi.
Bakalov and Korobov (1998)	Hfs levels of antiprotonic helium, $^4He^+\bar{p}$.
Bieroń et al. (1998)	E2 hfs of $4d5s^2$ levels of Y. $Q(^{90}Y)$ -125(11) mb.
Bouazza et al. (1998)	Zr I $(4d+5s)^4$ hfs. $Q(^{91}Zr)$ -230(20) mb.
Crespo Lopez Urrutia et al. (1998)	Observe M1 hfs transition of H-like Re. QED corrections from Shabaev (1994) a few tenths of per cent. Bohr-Weisskopf effects extracted.
Esquivel et al. (1998)	M1 hfs of Li, $2s^1$.
Godefroid et al. (1998)	Review on atomic structure calculations.
Gustavsson and Mårtensson-Pendrill (1998a)	Review on hyperfine anomalies (nuclear volume effects on M1 hfs).
Gustavsson and Mårtensson-Pendrill (1998b)	Nuclear magnetic moments should be remeasured. Present diamagnetic screening corrections for bulk are too inaccurate. Better values will enable QED tests on highly-ionized atoms.
Karpeshin et al. (1998)	TP between hfs levels of the H-like $^{229}Th^{89+}$. ($I=5/2$ nuclear ground state and $I=3/2$ 3.5 eV isomer). The 28 MT magnetic field at nucleus mixes the *nuclear* states.
O'Malley and Beck (1998)	M1 hfs of Sn^-, $5p^3$.
M. S. Safronova et al. (1998)	M1 and E2 hfs of Na-like systems, Z=11-16.
Shabaev (1998b)	TP between M1 hfs levels of H-like ions related to the bound-electron g-factor.
Shabaev et al. (1998e)	Ground-state M1 hfs splitting and lifetime for Li-like ions, Z=49-83. Includes QED.
Sunnergren et al. (1998)	Radiative corrections to M1 hfs of H-like systems.
Tomaselli et al. (1998)	M1 $1s$ hfs in H-like atoms with one-hole nuclei. ^{165}Ho...^{207}Pb.
van Lenthe et al. (1998)	M1 hfs of Cu-Au at DFT level. R/ZORA/NR.
Bieroń et al. (1999a)	E2 hfs of $3d^24s$ and $3d^3$ Ti^+. $Q(^{49}Ti)$ 247(11) mb.
Bieroń et al. (1999b)	M1 and E2 hfs of $2s$ and $2p$ states of Be^+, F^{6+}.
Derevianko et al. (1999b)	Off-diagonal, $6s-7s$ M1 hfs in Cs.
Kozlov and Porsev (1999)	M1 and E2 hfs of low-lying levels of Ba.
Norquist et al. (1999)	M1 and E2 hfs of Ru^-. MCDF.
Porsev et al. (1999a)	M1 and E2 hfs for low-lying levels of Yb.
M. S. Safronova et al. (1999)	M1 hfs of alkali atoms, Na-Fr.
Shabaev (1999)	Hfs of highly charged (H- and Li-like) ions. By combining them, nuclear factors can be eliminated. TP. QED included.

Table 5.9: Average radii and magnetic g-factors.

Reference	Comments
Moss and Sadler (1986)	Electric quadrupole moments of one-electron atoms. In $j = \frac{1}{2}$ states due to hfs. Resolves earlier inconsistencies.
L. Liu and Li (1991b)	Amplitudes of wave functions at nuclei for ions.
Anthony and Sebastian (1993)	Relativistic corrections to g-factors of He-like systems.
Fricke et al. (1993)	Radii for atoms and ions of Ta, E105 (Db).
Lindroth and Ynnerman (1993)	g-factors for Li, Be^+, Ba^+.
Marketos (1993)	Alkali atom g-factors. Li-Cs.
J. Persson (1993)	g-factors of np^2 systems.
Dzuba et al. (1994)	g-factors in Dy.
L. Liu et al. (1994)	Amplitudes of wave functions at nuclei for ions. DS.
Yan (1994)	g-factor ratio for ^{3}He and ^{4}He in the 2 $^3S_1$ state.
Yan and Drake (1994)	g-factors for helium 2 $^3S_1$, ^3P_J, $^1P_1$ and 3 ^3P_J states.
W. Huang et al. (1995)	Ne I excited levels.
Land and Horwitz (1995)	Zeeman effect for a relativistic bound state.
Seth et al. (1995)	Trends of atomic orbital energies and radii for Groups 11 (Cu-E111) to 15 (As-E115). Relativistic and shell-structure effects.
W.-Y. Liu et al. (1996)	Rydberg levels of Cs in strong magnetic field.
Gonzalo and Santos (1997)	Radiative corrections to Zeeman effect of 2 ^3P states of He.
Persson et al. (1997a)	Radiative corrections to electron g-factor in H-like ions.
Beck (1998)	Cs II $5p^-$ $6p$ level g-factors.
Shabaev (1998b)	TP between M1 hfs levels of H-like ions related to the bound-electron g-factor.
van Lenthe et al. (1998)	g-factors of Cu-Au at DFT level. R/ZORA/NR.
E. Johnson et al. (1999)	Ionic radii from $\langle r^n \rangle$ for M^q; M=Cr-Sg(E106); q=4+ to 6+.
Labzowsky et al. (1999a)	Relativistic and QED corrections to ns electron g factors of neutral K-Fr, Ba^+.

Table 5.10: Compton profiles, momentum distributions and spin densities.

Reference	Comments
Bergstrom et al. (1993)	Compton scattering from bound electrons in a fully relativistic independent-particle approximation.
Timms and Cooper (1993)	Electron momentum distribution in Pb.
Scherer et al. (1994)	Low-energy Compton scattering by a Dirac proton with anomalous magnetic moment. FW used.
Rocchi and Sacchetti (1995)	Radiative corrections to Compton cross section.

Table 5.11: Photon scattering, photoionization, x-ray scattering factors. Radiative recombination (the inverse photoelectric effect).

Reference	Comments
Gorshkov et al. (1967)	Screening effects in K-shell photoionization.
Mikhailov and Polikanov (1968)	Central potential. PT by reducing the Dirac equation to a Riccati equation. Used for K-shell relativistic photoeffect.
Boyle et al. (1993)	Photoionization cross section of atomic W.
T.-N. Chang (1993)	MBPT of atomic structure and photoionization.
S. H. Kim (1993)	Thomson scattering by a relativistic electron.
Kotochigova and	Multiphoton ionization and autoionization of Si I.

Reference	Comments
Lambropoulos (1993,1994)	
Kutzner et al. (1993)	Inner-shell photoionization of alkaline earth atoms.
Z. W. Liu and Kelly (1993)	Multiphoton ionization in strong laser fields.
J. Luo et al. (1993)	Scattering operator for elastic and inelastic resonant x-ray scattering. Applied on Ln, An, TM.
Pratt and Kim (1993)	Non-dipolar effects in atomic photoionization.
Schaphorst et al. (1993)	Multielectron inner-shell photoexcitation of Kr.
Tulkki (1993)	Outer-shell photoionization of Ar, K^+, Ca^{2+}. Combined effect of relaxation and channel interaction.
Verner et al. (1993)	Subshell photoionization cross sections of He-Zn.
Basavaraju et al. (1994)	Elastic scattering of 81-keV γ rays.
Chi and Huang (1994)	Photoionization of Mg.
Crawford and Reiss (1994)	Stabilization of relativistic photoionization by circularly polarized light.
Kutzner and Radojevic (1994)	Relaxation and interchannel coupling in inner-shell photoionization of atomic Yb.
Kutzner et al. (1994)	Inner-shell photoionization of Group 12 atoms.
Kutzner and Vance (1994)	Photoionization of Pd.
L'vov and Milstein (1994)	Elastic scattering of photons in a Lorentz scalar potential. Virtual spin-0 particle-antiparticle pairs involved
Rao et al. (1994)	L x-ray fluorescence, Z=46-51.
Rez et al. (1994)	DF x-ray scattering factors. $Z = 2 - 92$.
Ron et al. (1994)	Relativistic, retardation and multipole effects in photoionization cross sections. Z, n, and l dependence.
Shabaev (1994b)	QED theory of electron recombination with highly charged ions.
Tseng (1994)	Pair production by photons near threshold. Positron energy spectrum for Z=1-82.
C.-M. Wu et al. (1994)	Photoionization of Sr above $5p_{3/2}$ threshold. MC RRPA.
Filipponi and Di Cicco (1995)	K-edge X-ray absorption of Mo, Rh→Sn. EXAFS.
R. N. Lee and Milstein (1995); R. N. Li and Mil'shtejn (1995)	Delbrück scattering in a screened Coulomb field.
Y. Liu et al. (1995)	Photoexcitation of Ni $3p$ level. SO, exchange, hybridization.
Miecznik et al. (1995)	SO effects in photoionization of Al I.
Pratt and LaJohn (1995)	Multipoles beyond dipole in photoionization.
Rao et al. (1995)	M x-ray fluorescence, Z=78-92.
Tseng (1995)	Pair production by photons near the $2mc^2$ threshold. Energy-angle distribution. Z=1 ... 82.
Yoo et al. (1995)	Photoionization of Bi.
Froelich and Weyrich (1996)	Relativistic corrections to inelastic scattering of photons by atomic electrons.
Ichihara et al. (1996)	Radiative electron capture and photoelectric effect at high energies. Bare projectile, low-Z atom.
Keitel (1996)	Ultra-energetic electron ejection in relativistic atom. Laser field interaction.
Meyerhofer et al. (1996)	Relativistic mass-shift effects during high-intensity laser–electron interactions. Multiphoton scattering.
J.-H. Wang et al. (1996)	X-ray scattering factors for He-Ar. DF.

Reference	Comments
Chi (1997)	Near-threshold photoionization of Mg.
Donnelly et al. (1997)	$3p$ photoabsorption of Cr^+.
Kylstra et al. (1997)	1D Dirac model atom in an intense laser field.
Rao et al. (1997)	Rayleigh and Compton scattering cross sections for low, medium and high Z and $23.18 \leq E \leq 30.85$ keV.
Z.-W. Su and Coppens (1997)	X-ray elastic scattering factors. Z=1-54.
Tseng (1997b)	Pair-production polarization correlations of intermediate-energy photons on atoms.
Bhatia and Drachman (1998b)	Optical properties of helium, including BP-level relativity.
J.-J. Chang (1998)	Similarities between Dirac-Coulomb and Schrödinger-Coulomb radial functions. Photoionization of H.
Donnelly et al. (1998)	$3p$ photoabsorption of Mg^+.
Eichler et al. (1998)	Alignment caused by photoionization and in radiative electron capture into excited states of high-Z H-like ions.
Gorczyca et al. (1998)	SO effects in the photoionization excitation of Ne.
Kahane (1998)	Incoherent photon scattering functions. Z=1-110. DF.
Lagutin et al. (1998)	Relativistic effects in inner-shell atomic photoabsorption.
J. C. Liu et al. (1998)	SO components of resonant satellite photoionization of Ca^+.
Matrasulov (1998,1999)	Chaotic ionization of an H-like atom in intensive monochromatic field.
Mohan et al. (1998)	Ground-state photoionization of Ne-like Fe XVII.
Mohr (1998)	QED and the fundamental constants.
Wills et al. (1998)	SO effects in parity-unfavoured photoionization of Ne. Doubly excited resonances.
H. L. Zhang (1998)	Relativistic calculations of photoionization cross sections. He-like, Li-like systems.
Brinzanescu et al. (1999)	Radiative recombination: exact relativistic theory and the NR dipole approximation. Results for naked Ne and U nuclei.
Chakraborty et al. (1999)	Near-threshold photoionization for Ne-like systems, $Z = 10 - 15$.
Derevianko et al. (1999c)	Photoelectron angular distribution, He-Xe. Non-dipole effects.
Haque et al. (1999)	Photoionization of Ne-like Fe.
Haque and Pradhan (1999)	Photoionization Mg-like Fe.
Ionescu et al. (1999)	Inner-shell photoionization at relativistic energies. Vacuum-assisted processes most probable at high E. 'Vacuum spark'.
V. K. Ivanov et al. (1999)	Many-body effects in negative ion photodetachment. Review.
Krainov (1999)	Tunneling ionization of atoms by intensive laser radiation. Electron energies and angular distributions.
Luc-Koenig et al. (1999)	Multiphoton ionization dynamics of Ba. Raman couplings, dynamical Stark shifts.
Panek et al. (1999)	Electron scattering in powerful laser field. Angular and polarization effects. Electron handled as laser-dressed KG particle.
Trail and Bird (1999b)	Accurate structure factors from PP methods. Si.
Vrejoiu et al. (1999)	Retardation corrections to angular distributions of free-bound photoionization transitions in H-like atoms.
L.-R. Wang et al. (1999)	Doubly excited states in photoionization of Zn. Autoionization resonances.

Table 5.12: Electron and positron scattering. Dielectronic recombination.

Reference	Comments
Fontes (1992); Fontes et al. (1993a)	Effect of the generalized Breit interaction on electron-impact excitation cross sections.
Bartschat (1993); Bartschat et al. (1994)	Low-energy electron scattering from Cs.
Bettega et al. (1993, 1995)	MH_4 molecules; M=Ge-Pb. Electron scattering, elastic and inelastic. Local-density norm-conserving PP used.
Braidwood et al. (1993)	Satellite structure of Xe valence shell by electron-momentum spectroscopy.
M. H. Chen (1993b)	Dielectronic recombination for Ni-like Ta.
M. H. Chen and Reed (1993a)	Electron-impact ionization of Kr^{24+}, Kr^{25+} and Xe^{43+}.
M. H. Chen and Reed (1993b)	Effect of relativity and M2 transitions on the resonance contribution to electron-impact ionization. Li-like ions, Z=18...54.
Fontes et al. (1993b)	Method for electron-impact ionization for ions of any complexity.
Furst et al. (1993)	SO effects in excitation of noble gases by spin-polarized electrons.
C. Hofmann et al. (1993)	Distorted-wave scattering solution of Dirac electron from a Coulomb potential.
Hou et al. (1993)	Elastic electron or positron scattering from Ar.
Ivanov et al. (1993ab)	QED-based theory of decaying atomic states. Application for electron-collision strengths. Ne-like ions.
Khare and Raj (1993)	Elastic electron scattering by Ar. Spin polarization.
Koike (1993)	Inelastic electron scattering by Ln and An atoms. Quadrupole interaction important. Analogy to molecular rotation.
Kuo et al. (1993)	Positron-impact ionization of H-like ions.
Popov and Kuz'mina (1993ab)	Eikonal approximation for relativistic (e,2e) experiments.
Qiu et al. (1993)	Dielectronic recombination for Ne-like Ti from low-lying F-like states.
Raeker et al. (1993)	Charge-cloud distribution of heavy atoms after excitation by polarized electrons. Hg, Tl.
Reed and Chen (1993)	Polarization of line emission from H-like and He-like ions, following electron impact.
Salvat and Mayol (1993)	Partial wave analysis for electron and positron elastic scattering. Program.
Srivastava et al. (1993)	Electron-impact excitation of Hg.
Szmytkowski (1993a)	Low-energy positron scattering on alkaline-earth atoms.
Szmytkowski (1993b)	Elastic positron scattering from Hg.
Szmytkowski (1993c)	Elastic positron scattering from Zn and Cd.
Thumm (1993)	Dirac R-matrix method for scattering of slow electrons from alkali-metal-like targets.
Thumm et al. (1993)	Relativistic effects in spin polarization for low-energy electron-Cs scattering.
Thumm and Norcross (1993)	Angle-differential and momentum-transfer cross sections for low-energy electron-Cs scattering.
J.-M. Yuan and Zhang (1993a)	Spin polarization of electrons, elastically scattered from Ar in the Ramsauer-Townsend region.
J.-M. Yuan and Zhang (1993b)	Spin polarization of electrons, elastically scattered from alkaline earth atoms in the Ramsauer-Townsend and low-lying shape resonance regions.

Reference	Comments
H. L. Zhang and Sampson (1993)	Improvements of distorted-wave approach to electron impact excitation of ions.
Ast et al. (1994)	Electron-impact K-shell ionization of Ag, Au.
Baluja and Gupta (1994)	Electron scattering from iron at 10-5000 eV.
Bartschat (1994)	Low-energy electron scattering from Tl.
Berrington (1994)	Electron-impact excitation of Be-like systems, Z=4-28.
M. H. Chen and Reed (1994)	Angular distribution of Auger electrons after electron-impact ionization. Be-like ions, Z=12...42.
M. H. Chen et al. (1994)	Effect of Coster-Kronig transitions on electron-impact excitation rates for F-like ions.
W.-Y. Cheng and Huang (1994a)	Polarization correlations of radiation from electron-impact excited atoms.
Dasgupta and Whitney (1994)	Z-scaled data for dielectronic recombination from O-like to F-like ions.
Dzuba and Gribakin (1994)	Correlation-potential method for electron scattering.
Faulkner (1994)	Scattering matrices for non-spherical SR potential.
Fontes et al. (1994)	Effect of generalized Breit interaction on electron-impact excitation cross sections.
Glass (1994a)	Relativistic continuum distorted wave theory for electron capture.
Glass (1994b)	Asymmetric theories of relativistic electron capture.
Johnson and Guet (1994)	Elastic electron scattering from Xe,Cs^+,Ba^{2+}.
Keller and Whelan (1994)	Plane wave Born approximation for relativistic (e,2e) processes.
Keller et al. (1994)	Distorted-wave Born approximation for inner-shell (e,2e) processes.
Khare et al. (1994)	L3-shell ionization of Xe and Au by electron and positron impact.
Kumar et al. (1994a)	Electron scattering from Zn and Pb. Spin polarization and cross sections.
Kumar et al. (1994b)	Electron scattering from heavy alkaline earths.
Rez et al. (1994)	DF mean inner potential for electron scattering. $Z = 2 - 92$.
Rosenberg (1994a)	Infrared radiative corrections to potential scattering of a Dirac electron.
Rosenberg (1994b)	Minimum principle for potential scattering of Dirac electron.
Szmytkowski (1994)	Elastic positron scattering from Kr and Xe.
Szmytkowski and Sienkiewicz (1994a)	Spin polarization of slow electrons, elastically scattered from Zn-Hg.
Szmytkowski and Sienkiewicz (1994b)	Spin polarization of slow electrons, elastically scattered from Xe.
Szmytkowski and Sienkiewicz (1994c)	Spin polarization of slow electrons, elastically scattered from Sr, Ba.
Tang and Dorignac (1994)	Electron scattering factors for High-resolution electron microscopy (HREM) image simulation. DS potential.
H.-G. Teng et al. (1994a)	Dielectronic recombination of He-like systems.
H.-G. Teng et al. (1994b)	Dielectronic recombination of F-like systems.
S. Wang et al. (1994)	Cross sections for electron scattering by ground-state Ba. Elastic scattering and $6s6p\ ^1P_1$ excitation.
Young and Norrington (1994)	Solution of relativistic asymptotic equations in electron-ion scattering. Program.
Zeman et al. (1994a)	Relativistic distorted-wave calculation of electron impact excitation of Cs.
Zeman et al. (1994b)	Intermediate energy electron impact excitation of Cs.

Reference	Comments
H. L. Zhang and Pradhan (1994)	Electron-impact excitation. B-like ions. Z=8 ... 26.
H. L. Zhang and Sampson (1994a)	Electron-impact collision strengths for B-like ions, Z=8-92. $\Delta n = 0, n = 2$.
H. L. Zhang and Sampson (1994b)	Electron-impact collision strengths for B-like ions, Z=8-92. $n = 2$ - $n = 3$.
Baylis and Sienkiewicz (1995)	Represent electron-scattering polarization data by 'polarization trajectories' on a Poincaré sphere.
M. H. Chen and Scofield (1995); M. H. Chen and Scofield (1998)	Relativistic effects on angular distribution and polarization of dielectronic satellite lines of H-like ions, Z=9...92.
Fontes et al. (1995)	Electron-impact ionization cross sections for $U^{90+,91+}$.
Horbatsch and Shapoval (1995b)	Relativistic two-particle scattering resonances in the Tamm-Dancoff approximation.
Khare and Wadehra (1995)	K-shell ionization by electron impact.
Kisielius et al. (1995)	Electron-impact excitation of H-like ions.
Mohan et al. (1995)	Electron-impact FS transitions in Cu XX.
Moores and Reed (1995abc)	Electron-impact ionization of high-Z H-like to Be-like ions.
Pindzola et al. (1995)	Photorecombination of highly charged U ions. (Inverse photoionization: $e^- + U^{90+} \rightarrow U^{89+}(1s^2 2s) + h\nu$).
Prinz et al. (1995)	SO effects of the continuum electrons in (e,2e) experiments.
Rosenberg (1995)	Electron scattering by heavy hydrogenic ion.
Srivastava et al. (1995a)	Excitation of the $np^5(n+1)p\ ^3D_3$ states of Ar-Xe by spin-polarized electrons.
Srivastava et al. (1995b)	Electron excitation of Yb.
Srivastava et al. (1995c)	Electron excitation of Cu.
Szmytkowski (1995)	Relativistic multi-channel variable phase method for asymptotic equations of electron-atom and electron-ion scattering.
Whelan et al. (1995)	Triple differential (e,2e) cross sections for Au and U at relativistic impact energies.
J.-M. Yuan (1995)	Low-energy electron scattering from Ca-Ba, Yb. Intra-atomic relativistic effects.
Zeman et al. (1995a)	Electron impact excitation of Cs.
Zeman et al. (1995b)	Test of LS approximation for electron-impact excitation of Cs.
H. L. Zhang and Pradhan (1995a)	Relativistic and radiation damping effects in electron-impact excitation of highly charged ions.
H. L. Zhang and Pradhan (1995b)	Relativistic and electron-correlation effects in electron-impact excitation of Fe^{2+}.
H. L. Zhang and Sampson (1995)	Relativistic collision strengths for optically allowed $\Delta n = 0$ transitions between magnetic sublevels of highly charged ions. Extremely large angular momenta (of order of 190) needed for the free electron.
Ait-Tahar and Grant (1996)	B-like Fe. Dirac R-matrix approach.
Ast et al. (1996)	Binary peak in (e,2e) collisions.
G.-X. Chen (1996);G.-X. Chen and Y.-B. Qiu (1997b)	Fully relativistic distorted-wave Born procedure for electron-impact ionization. Ni-like Gd, U.
Keller et al. (1996a)	Relativistic 1st-order Born approximation for inner-shell (e,2e) processes.
Keller et al. (1996b)	(e,2e) processes with spin-polarized electrons.

Reference	Comments
McCann et al. (1996)	Energy dependence of relativistic nonradiative electron capture.
Srivastava et al. (1996a)	Excitation of the 6 $^{1,3}P_1$ states of Hg by polarized electrons.
Srivastava et al. (1996b)	Excitation of the 5 $^{1,3}D_2$ states of Cd by polarized and unpolarized electrons.
Zeman et al. (1996)	Relativistic effects of generalized Stokes parameters for electron impact excitation of one valence electron atoms.
Ait-Tahar et al. (1997)	Cs. Dirac R-matrix approach.
Cai et al. (1997)	Electron-impact excitation of Cu-like ions, $Z \leq 82$.
G.-X. Chen and Qiu (1997a)	Electron-impact ionization of F-like Se.
Ehlotzky et al. (1997)	Review on electron-atom collisions in laser fields.
El Messaoudi et al. (1997)	K-shell ionization by electron impact. Effect of Breit interaction.
Kaur et al. (1997)	Electron-impact excitation of Mg and Zn.
Keller and Dreizler (1997)	Triply differential cross sections for electron-atom bremsstrahlung.
Labzowsky et al. (1997b)	Non-resonant QED corrections to radiative electron capture of highly charged ions.
Pelc and Horwitz (1997)	Complete sets of states in relativistic scattering theory.
Pindzola and Griffin (1997)	Electron-impact ionization of W ions.
Schaffer and Pratt (1997)	Relativistic partial-wave calculations of triply differential electron-atom bremsstrahlung.
Sienkiewicz and Baylis (1997)	Spin polarization of slow electrons, elastically scattered by Kr.
Tseng (1997a)	Unpolarized triply differential cross section of electron bremsstrahlung. Z=13,79.
Whelan et al. (1997)	Relativistic, energy-sharing (e,2e) collisions in coplanar constant $\Theta_{1,2}$ geometry.
Zeman et al. (1997)	Relativistic calculation of superelastic electron-alkali atom scattering.
H. L. Zhang and Sampson (1997)	Collision strengths for $(n = 2) - (n = 3)$ transitions in C-like ions, Z=9-54.
Ancarani et al. (1998)	Effect of Coulomb boundary conditions for (e,2e) processes on the K-shell.
C. Y. Chen et al. (1998)	Electron-impact ionization of Ne-like ions, $22 \leq Z \leq 39$.
G.-X. Chen and Ong (1998b)	Electron-impact excitation of Fe XXIII.
G.-X. Chen and Ong (1998c, 1999a)	Electron-impact excitation of F-like Se.
J. N. Das and Dhar (1998)	Triple differential cross sections of K-shell ionization by electrons for medium-heavy atoms.
C.-Z. Dong et al. (1998)	Dielectronic recombination of Fe^{25+}.
Fontes (1998)	Electron-impact ionization of lowest $J = 0, 2$ levels of Kr, Xe. Role of the $5p^5 5d$ configuration and SO coupling.
Griffin et al. (1998)	R-matrix electron-impact excitation cross sections in intermediate coupling: MQDT approach.
Keller et al. (1998)	Three-body effects in relativistic (e,2e) processes.
Keller and Dreizler (1998)	Interpretation of (e,2e) experiment in coplanar asymmetric geometry.
Mazevet et al. (1998)	Semirelativistic DWBA for ionization of closed-shell atoms at intermediate energies.
Y.-Z. Qu et al. (1998)	Dielectronic recombination for H-like systems, Z=2-79.

Reference	Comments
Sauter et al. (1998)	Spin asymmetry in (e,2e) processes. Z-dependence. Cu, Ag, Au.
Zeman et al. (1998)	Relativistic distorted-wave calculation of inelastic electron-alkali atom scattering.
Badnell and Griffin (1999)	Correlation resonances in electron-impact excitation of Ni^{4+}.
Beier et al. (1999)	QED effects on radiative electron capture.
G.-X. Chen and Pradhan (1999)	Electron-impact excitation of Fe^{5+}.
Fontes et al. (1999a)	Fully relativistic $1s$ ionization cross sections.
Fontes et al. (1999b)	Fully relativistic $2s, 2p$ ionization cross sections. $Z - N \geq 3, Z \leq 92, N \leq 12$.
Fontes et al. (1999c)	Effect of generalized (energy-dependent) Breit interaction on electron-impact ionization to specific magnetic sublevels. Large for Xe.
J. F. Gao et al. (1999)	Direct and indirect relativistic effects on electron scattering from Cs and Au atoms. ('Direct' for incident electron, 'indirect' for atomic electrons.) Direct found more important for Cs, indirect for Au.
Griffin et al. (1999)	Electron-impact excitation of Mg-like ions.
X.-Z. Guo et al. (1999)	Low-energy electron-impact excitation of Kr $4p^5 5s$. Sensitive to relativistic effects in target.
Nefiodov et al. (1999b)	QED effects of radiative interference in recombination of electrons with heavy multicharged ions. Dielectronic recombination of He-like U.
H. L. Zhang and Sampson (1999)	Collision strengths for the 105 Δn=0 transitions with $n = 2$ in the N-like ions, Z=12-92.

Table 5.13: Particle-atom collisions.

Reference	Comments
Cusson et al. (1985)	Time-dependent 3D Dirac equation in heavy-ion scattering.
Hofstetter et al. (1992)	Ionization of hydrogen by relativistic heavy projectile.
Porter (1992)	High-velocity projectile-z^3 term in modified Bethe-Bloch stopping-power theory. (z projectile nuclear charge).
Avdonina and Pratt (1993)	Bremsstrahlung from ions in a model potential.
Baltz et al. (1993)	Pair production in heavy-ion collisions.
Dzuba et al. (1993)	Interaction between slow positrons and atoms. Ne-Rn.
Ichihara et al. (1993)	Electron capture in relativistic atomic collisions. Single-electron targets and bare projectiles.
Kürpick et al. (1993,1995abc)	Ion-atom collisions using molecular codes.
Musakhanov and Matveev (1993)	Inelastic collisions of multiply charged ions with atoms.
De Cesare et al. (1994)	^{4}He-ion induced L-shell ionization, Z=46-70.
Halabuka et al. (1994)	Inner (L,M) shell ionization by heavy projectiles. DF.
V. I. Matveev and Musakhanov (1994ab)	Inelastic collisions of multicharged ions with atoms.
Šmit and Orlić (1994)	Adiabatic L-shell ionization by protons.
Baltz (1997)	Exact Dirac calculation of ionization and pair production induced by ultrarelativistic heavy ions.
Ghilencea et al. (1994)	Coulomb Born approximation for double Bremsstrahlung.
Deco et al. (1995)	Scattering involving Coulomb potentials. Ion-atom collisions.

Reference	Comments
Halabuka et al. (1995)	Proton-induced alignment. DF.
Momberger et al. (1995)	Numerical, momentum-space solution of time-dependent Dirac equation for Au^{79+} or U^{92+} impinging on U^{91+}.
Dzuba et al. (1996a)	Positron scattering and annihilation. H, He-Xe.
Ichihara et al. (1996)	Radiative electron capture and photoelectric effect at high energies. Bare projectile, low-Z atom.
Kürpick (1996)	High-energy H^+-Ne collision handled using molecular DF-LCAO code.
Lindhard and Sørensen (1996)	Relativistic theory of stopping for heavy ions.
Vargas et al. (1996)	Electronic energy loss of low-energy protons, channeled in single-crystal Au ⟨100⟩ direction.
Moiseiwitsch (1997)	Virial theorem for electron capture from H-like atom.
X. Feng et al. (1998)	Positron scattering from Rb, Cs. Relativistic close-coupling calculations. DF bound states.
Fricke et al. (1998)	Review on ion-atom and ion-solid collisions.
Pivovarov (1998)	Coherent excitation of H-like heavy ions penetrating through a crystals.
V. I. Matveev and Matrasulov (1999)	Single and double K-vacancy production by collision with highly charged ions.

Table 5.14: Atom-atom collisions and interatomic potentials.

Reference	Comments
Ichihara et al. (1993)	Electron capture in relativistic atomic collisions. Single-electron targets and bare projectiles.
Marinescu et al. (1994a)	Interaction of two alkali atoms. Includes retardation.
J. Thiel et al. (1994,1995)	Electron-positron pair creation in relativistic heavy-ion collisions.
Eichler and Meyerhof (1995)	Relativistic atomic collisions. Book.
Thumm et al. (1995)	Highly-charged ion–C_{60} collisions. DS.
Kunz et al. (1996)	Hg-Hg interaction potential. Damped dispersion +repulsion. DK.
Alscher et al. (1997)	Electron-positron pair production in heavy-ion collisions.
Hickman et al. (1997)	FS effects in O^+-O collisions.
Khabibullaev et al. (1998)	Inelastic collisions of relativistic highly charged ions with heavy atoms. K-vacancy production.
Marinescu et al. (1998)	Francium-francium potentials, C_n.
Segev and Wells (1998)	Pair production in ultrarelativistic heavy-ion collisions.
Busic et al. (1999)	Electron-positron production with electron capture. U^{92+}-U^{92+}.
Ionescu and Belkacem (1999)	Relativistic collisions of highly-charged ions.
Schulze et al. (1999)	Time evolution of QED vacuum solved numerically.
	MO x-ray spectra in U^{92}–Pb collisions.

Table 5.15: Nuclear and mesonic processes involving electronic wave functions.

Reference	Comments
Band et al. (1992a)	Internal conversion in ^{229}Pa.
Band and Trzhaskovskaya (1993a)	Internal conversion at $E_\gamma = 72$ keV in Re-187.
Band and Trzhaskovskaya (1993b)	Internal conversion coefficients for 35 low-energy nuclear transitions with $E_\gamma \leq 3$ keV.
Watanabe et al. (1993)	Electron energy spectrum and asymmetry in decay of bound 1s muons. ^{16}O ... ^{209}Bi.

Reference	Comments
Greub et al. (1995)	Decays of muonic and pionic atoms into electronic atoms are enhanced by high Z. For Z=80, the relativistic increase is a factor of 50.
C. R. Hofmann and Soff (1996)	Internal-pair creation in extended nuclei.
Yamanaka and Ichimura (1999)	Nuclear polarizability contributions to $1s$ energies of H-like ^{208}Pb and ^{238}U. Transverse polarization is even more important than longitudinal one.

Table 5.16: Parity-violation effects in atoms and molecules.

Reference	Comments
Lewis and Blinder (1975)	Stark-induced anapole magnetic fields in atoms. (Anapole = PNC-induced nuclear moment of wrong parity.)
Flambaum (1993)	Dynamic enhancement of PNC in systems with a dense spectrum of excited states.
Flambaum and Hanhart (1993)	Magnetic interaction between R atomic electrons and PNC nuclear moments.
Flambaum and Sushkov (1993); Sushkov (1993)	Proposed observation of nuclear anapole moments as NMR shifts in a laser beam.
Johnson et al. (1993)	PNC in atomic Cs.
Khriplovich (1993)	Fundamental symmetries in atomic physics.
Mårtensson-Pendrill (1993b)	PNC effects in atomic systems.
Pindzola (1993)	Parity-violation effects on Auger-electron emission from highly charged atomic ions. $2s^2$ $J = 0$ of U^{90+}.
Sandars (1993)	P and/or T violation. Review.
Dzuba et al. (1994)	P- and PT-odd weak interactions in Dy.
Kozlov and Ezhov (1994); Kozlov (1997)	YbF. Dipole moment of the odd electron.
Shukla et al. (1994a)	Atomic Rb.
Shukla et al. (1994b)	CC calculation of PT violation in atoms and molecules.
Bednyakov et al. (1995)	Parity-conserving weak interactions for highly charged ions. For Z=83 $1s$, 10^{-5} and 10^{-7} eV for Lamb shift, M1 hfs, respectively.
Dzuba et al. (1995)	PNC in Fr.
Kozlov and Labzowsky (1995)	PNC in diatomics. MF; M=Ba,Yb,Hg,Tl,Pb.
Kulkarni et al. (1995)	Relativistic mean-field approach to anapole moment. Atomic, parity-violating hyperfine transitions.
Malhotra et al. (1995)	PNC in Ba^+.
Schäfer and Reinhardt (1995)	VP as test of C and CPT invariance. Muonic $4f_{7/2}$ and $5g_{9/2}$ levels in ^{209}Pb.
Dunford (1996)	PNC in high-Z He-like ions.
Funakubo et al. (1996)	Numerical approach to CP-violating Dirac equation.
Sapirstein (1996b)	PNC effects in atoms.
Kozlov et al. (1996)	Nuclear anapole moment and the M1 transitions in Bi.
Kozlov and Yashchuk (1996)	P- and PT-odd effects in diatomic van der Waals molecules.
Maul et al. (1996)	Prospects for PNC experiments with highly charged ions.
Titov et al. (1996)	YbF. P,T-odd spin-rotational Hamiltonian.
Bouchiat and Bouchiat (1997)	Review on parity violation in atoms.
B. P. Das (1997)	PNC E1 transition of Yb.
Dzuba et al. (1997a)	PNC in Cs.

Reference	Comments
Flambaum and Murray (1997)	A radial (monopole) magnetic field can induce a T-invariance-violating electric dipole moment. Xe, Cs, Hg, Tl. TlF, HgF, YbF.
Khriplovich and Lamoreaux (1997)	CP violation without strangeness.
Kozlov et al. (1997)	Enhancement of the electron dipole moment in BaF.
Laerdahl et al. (1997b); Quiney et al. (1998a)	TlF. PT-odd interactions. DF.
Lazzeretti and Zanasi (1997)	PNC in HEEH; E=O,S.
Parpia (1997)	TlF. DF.
Zolotorev and Budker (1997,1999)	PNC in relativistic hydrogenic ions. Circular dichroism on the $1s \rightarrow 2s$ transition due to interference between the M1 and PNC-induced E1 amplitudes.
Bakasov et al. (1998)	Parity-violating potentials as function of structure for H_2O_2, H_2S_2, ... alanine. 'Electroweak quantum chemistry'. PT.
Bruss et al. (1998,1999)	PNC-induced energy shifts in inhomogeneous electric fields.
Ceulemans et al. (1998)	Molecular anapole moments
Geetha et al. (1998)	Nuclear-spin-dependent PNC transitions in Ba^+, Ra^+.
Kiyonaga et al. (1998)	1- and 2-electron SO contributions to PNC energy shifts of amino acids and helical alkanes.
Kulkarni et al. (1998)	Relativistic mean-field calculation of parity-violating observables in Fr.
Maul et al. (1998)	'Stark quenching' in laser fields for PNC observations. One- and two-photon transitions of Be-like $2s2p\ ^3P_0$ levels.
Mosyagin et al. (1998)	YbF molecule. Electron dipole moment experiment.
Parpia (1998)	YbF. DF.
Quiney et al. (1998b)	PT-odd effects in YbF $^2\Sigma$.
Zanasi and Lazzeretti (1998)	Stabilization of natural L-enantiomers of α-amino acids via parity-violating effects.
Bednyakov et al. (1999)	Electroweak radiative corrections.
Byrnes et al. (1999)	Enhancement of electron dipole moment for Au, Fr.
Flambaum (1999)	Large P and T invariance violation in Ra atom due to high Z, and close-lying even/odd states.
James and Sandars (1999)	Parametrized nuclear size and shape for atomic PNC.
Laerdahl and Schwerdtfeger (1999)	PNC for chiral molecules HEEH; E=O-Po. Z^5 behaviour. For a single heavy centre, as in HTeOH, the effect is small. DF.
Lazzeretti et al. (1999)	Stabilization of *d*-camphor via weak neutral currents.

Chapter 6

Symmetry

Table 6.1: Group theory and symmetry aspects.

Reference	Comments
Titov (1992)	Matrix elements of the $U(2n)$ generators in SO basis.
Fowler and Ceulemans (1993)	SO coupling coefficients for icosahedral molecules.
Hecht and Barron (1993)	Time-reversal and Hermiticity characteristics of polarizability and optical-activity operators.
Altmann and Herzig (1994)	Comprehensive point-group theory tables up to D_{10d}, I_h.
J. Meyer (1994)	Erratum to J. Meyer et al. (1989)[5277].
Aucar et al. (1995a)	Operator representations in Kramers bases.
Koizumi and Sugano (1995)	Geometric phase in two Kramers doublet molecular system.
Aucar (1996)	Time reversal asymmetry and ground-state average values.
Balasubramanian (1996)	The icosahedral double group, I_h.
Cao et al. (1996)	Use of symmetry in the DF method.
Jensen et al. (1996)	MCDF for molecules. Formalism. Incorporate time-reversal and D_{2h} symmetries.
J. Meyer et al. (1996)	New version of program TSYM by J. Meyer et al. (1989)[5277].
Visscher (1996)	Construction of double-group symmetry functions. D_2^*, D_{4h}^*.
Fleig et al. (1997)	Use of time-reversal symmetry between Kramers pairs in MC DK calculations, especially CASSCF.
J. Meyer (1997)	Addendum to J. Meyer et al. (1989)[5277].
Sjøvoll et al. (1997b)	Determinantal approach to SO CI. Time-reversal and double-group symmetry.
Kettle (1998)	Double, triple and quadruple groups. (The latter two correspond to 'spins' of 1/3 and 1/4, respectively).
Boya and Byrd (1999)	Clifford periodicity from finite groups.
La Cour Jansen et al. (1999)	Evaluation of SO matrix elements in a spin-adapted basis.
Saue and Jensen (1999)	Quaternionic symmetry in DF calculations. D_{2h} and subgroups.
Yabushita et al. (1999)	SO CI using graphical unitary group approach.

Chapter 7

Molecular Calculations

In this chapter we first list the technical developments by method. Finally, in Table 7.10, we review the molecular production calculations by the heavy element, or group of elements in the compound.

Table 7.1: One-electron systems.

Reference	Comments
Moss (1993a)	Rovibrational studies of HD^+. Includes R and QED^{3701} corrections.
Moss (1993b)	$2p\sigma_u$-$1s\sigma_g$ spectrum of D_2^+.
Moss (1993c)	Dito for H_2^+.
Rutkowski et al. (1993)	Relativistic virial theorem for diatomic molecules. H_2^+. Large-R and small-R limits.
Düsterhöft et al. (1994)	$NiPb^{109+}$.
Franke (1994)	Relativistic effects from Direct Perturbation Theory. Th_2^{179+}.
C. Müller (1994)	Finite-element solution of time-dependent Dirac equations.
Sundholm (1994)	Fully numerical (2D) solutions of 2nd-order Dirac equation for H_2^+, ... Th_2^{179+}, Fm_2^{199}. Accurate for small Z.
Momberger et al. (1995)	Numerical, momentum-space solution of time-dependent Dirac equation for Au^{79+} or U^{92+} impinging on U^{91+}.
Parpia and Mohanty (1995a)	H_2^+, H_3^{2+}, H_4^{3+}. Th_2^{179+}.
Pöschl and Dietrich (1995)	One-electron two-center Dirac problem using a diatomic basis of H-like spinors.
Cencek and Kutzelnigg (1996)	Accurate H_2^+.
Chauhan and Raina (1996)	High-energy electron scattering from two-centre potentials.
Gorvat et al. (1996)	One-electron two-centre Dirac problem.
Lazur et al. (1996abc)	The one-electron two-centre problem.
Molzberger and Schwarz (1996)	Effects of different order in α^2 on energies of H-like atoms. Compare Dirac with 1st- and 2nd-order DK.
W. H. E. Schwarz et al. (1996)	H_2^+. Interpretation of relativistic effects on chemical bonding.
Franke (1997)	One-electron systems using DPT.
V. I. Matveev et al. (1997)	LCAO solution of two-centre Dirac equation. Supercritical limit obtained.
LaJohn and Talman (1998)	Th_2^{179+}. A minimax STO solution.
Rutkowski et al. (1998)	DPT on H_2^+-like systems.
Alexander and Coldwell (1999)	Th_2^{179+}.
Balinsky and Evans (1999ab)	Stability of one-electron molecules. 'No-pair' Hamiltonian.
Matrasulov et al. (1999)	Dirac electron in the field of two opposite charges. $Z < 137$ and $Z > 137$ considered.
Rutkowski (1999)	Th_2^{179+} at $R = 2/90$ au. Several states. DPT.
Yan and Ho (1999)	Relativistic effects in positronium hydride (PsH, e^-e^+p).

The following Table 7.2 contains both DF-LCAO and fully numerical calculations. For further production results, see Table 7.10.

Table 7.2: Four-component, full Dirac calculations on molecules.

Reference	Comments
S. N. Datta (1993)	DF/HF comparisons for Li compounds.
Dyall (1993a)	DF/HF for MO; M=Ge-Pb. Comparisons with PP, PT.
Dyall (1993b)	PtH, PtH^+, PtH_2. DF/HF. Comparisons with PP, DK.
Ishikawa (1993)	Comment on 'segmented contractions' of relativistic Gaussian basis sets (Matsuoka (1992a), paper 5228).
Malli et al. (1993ab, 1994)	Universal Gaussian basis for DF calculations.

Reference	Comments
Mohr and Soff (1993)	Nuclear-size correction to electron SE. $1s, 2s, 2p_{1/2}$, $Z \leq 100$.
Pisani et al. (1993)	Discuss relativistic effects in atoms and molecules using LCAO calculations on H-like systems as example.
Visscher (1993,1994)	Correlated, fully relativistic methods.
L. Yang et al. (1993)	Fully numerical (FEM), fully relativistic H_2 to 10-figure accuracy at DF level.
Baeck and Lee (1994)	Effect of the magnetic part of the Breit term on the $^2\Pi$ states of hydrides (HX or HX^+; X=Be-F, Mg-S).
de Jong et al. (1994)	The MOLFDIR package.
Düsterhöft et al. (1994)	Numerical solution of Dirac equation for $NiPb^{109+}$.
Dyall (1994a)	Separation of spin effects for DCB Hamiltonian. Rg (Ne-Rn).
Dyall (1994b)	MP2 theory based on DF. Up to two open shells. O_2.
Dyall (1994c)	Review on DF/GTO for polyatomic molecules.
Kaldor and Hess (1994)	DK CC on Au, AuH.
Malli and Styszyński (1994)	ThF_4. DF.
Merenga and Andriessen (1994)	Improvement of MOLFDIR.
Nieuwpoort et al. (1994)	The MOLFDIR molecular code.
Pisani and Clementi (1994a)	DF calculations on closed-shell molecules. Hydrides.
Pisani and Clementi (1994b)	H_2E; E=O-Po. DF/HF.
Visscher et al. (1994)	The MOLFDIR package.
Dijkstra et al. (1995)	DF + Madelung potential model for $[EuO_6]^{9-}$ in crystals.
Kaldor (1995,1997)	Reviews on the Fock-space CC approach.
Kotochigova and Tupitsyn (1995)	Generalized Valence Bond approach, based on numerical DF basis orbitals. Large-R quasimolecules Na_2, In_2.
Minami and Matsuoka (1995)	GTO basis for $_{86}$Rn-$_{94}$Pu. DF.
Parpia and Mohanty (1995b)	H_2,HF,HCl,H_2O,NH_3,CH_4. DF/HF.
Pisani and Clementi (1995a)	HE; E=O-Po. DF/HF.
Pisani and Clementi (1995b)	DF calculations on closed- and open-shell molecules.
Saue (1995)	Four-component molecular methods. Thesis.
Visscher et al. (1995)	The MOLFDIR package.
Cao et al. (1996)	Use of symmetry in the DF method.
Dyall and Faegri (1996)	GTO basis for DF. Rn.
Jensen et al. (1996)	MCDF for molecules. Formalism. Incorporate time-reversal and D_{2h} symmetries.
Jorge et al. (1996,1997ab); Jorge and da Silva (1998)	GTO-basis sets.
Malli and Styszyński (1996)	UF_6. DF.
Mohanty and Parpia (1996)	AgH. DF/HF.
Saue et al. (1996)	DF on HX; X=I,At,E117.
Visscher (1996)	Construction of double-group symmetry functions.
Visscher et al. (1996a)	Relativistic, unrestricted CC method, including noniterative connected triples.
Dyall (1997); Dyall and Enevoldsen (1999)	'Normalized elimination of small components'. Can make light atoms non-relativistic.
Flocke et al. (1997abc); Flocke (1997)	Symmetric-group approach to relativistic CI.

Reference	Comments
Ishikawa et al. (1997)	Finite-nucleus models for GTO spinors.
Ladik (1997)	DF equations for solids.
Laerdahl et al. (1997a)	DF-based MP2. A 'direct' (no disk), Kramers-restricted code. CuF-AuF.
Merenga (1997)	Applications of MOLFDIR on cluster models of Ce-containing crystals.
Parpia (1997)	DF on TlF.
Saue et al. (1997)	Principles of direct (no disk) DF. Application on CsAu.
Sjøvoll et al. (1997a)	PdH. SO CI at DK level or DF level.
Tatewaki and Matsuoka (1997)	GdF. DF. Gd $5d \rightarrow$F $2p$ donation, F $2s$ - Gd $5p$ hybridization.
Visscher (1997)	Eliminate small-component integrals $(SS\|SS)$ by a simple point-charge correction.
Visscher and Dyall (1997)	DF atomic calculations using different nuclear charge distributions.
Visscher et al. (1997)	Relativistic RPA for frequency-dependent polarizabilities, $\alpha(\omega)$. H_2O, SnH_4, Hg.
de Jong (1998)	DF applications on I_2, UF_6, UO_2^{2+}.
Düsterhöft et al. (1998)	Numerical solution of Dirac-Slater equations for C_2.
Dyall (1998b)	Optimized DZ basis for $4p, 5p, 6p$ elements. Finite nucleus. DF/HF.
Hu et al. (1998)	Band-structure version of the DF code MOLFDIR. Application to a 1D chain of Se.
Ishikawa et al. (1998)	DF finite-field theory of NMR shielding.
Laerdahl et al. (1998)	DF (+MP2) for MF, MH, MH_3; M=La,Lu,Ac,Lr. Lanthanide and actinide contractions.
Malli and Styszyński (1998)	$RfCl_4$. DF.
Parpia (1998)	YbF. Unrestricted DF.
Quiney et al. (1998a)	TlF. DF. Small-r solutions for PNC purposes.
Quiney et al. (1998c)	H_2O. PT or self-consistent Breit term.
Skaane (1998)	Development and applications of the BERTHA code.
Watanabe and Matsuoka (1998)	DF with a frozen-core approximation. HI, ThO.
Dyall (1999)	ThO_2, PaO_2^+, UO_2^{2+}. Bonding and bending.
Hada et al. (1999)	HX;X=H,F-I. Proton NMR shifts.
Hu et al. (1999ab)	Fits of GTO basis functions. Hg, HgO, Se chain.
Kaldor and Eliav (1999)	High-accuracy calculations for heavy and superheavy elements.
Kullie et al. (1999)	DF-FEM on diatomics. H_2,LiH,BH,HF,N_2,CO,Ar,HCl.
Quiney et al. (1999)	The BERTHA molecular DF code. Review.
Saue and Jensen (1999)	Quaternionic symmetry in DF calculations. D_{2h} and subgroups.
Suzuki and Nakao (1999)	Fully relativistic LCAO approach for crystals. Au, InSb.

Table 7.3: Molecular all-electron calculations using 'no-pair' or other transformed Dirac Hamiltonians. Perturbation theories included.

Reference	Comments
Fraga and Karwowski (1974)	Two nuclear-mass-dependent terms in the BP equation. Of same order as the hyperfine interaction.
Klotz (1985)	Ab initio calculation of spin-forbidden transitions.
Bearpark et al. (1993)	SO interactions from SCF wave functions.
Dyall and Faegri (1993)	Finite-nucleus effects at PT level discussed.
Gould and Battle (1993ab)	Spin-dependent unitary-group approach to the BP Hamiltonian.
Pizlo et al. (1993)	The DK approach tested on Au and AuH.
Rohse et al. (1993)	H_2, H_3^+. DPT.
van Lenthe et al. (1993)	Relativistic regular two-component Hamiltonians. Tests on the U atom.
Dyall (1994a)	Separation of spin terms from the Dirac Hamiltonian.
Gleichmann and Hess (1994a)	DK tested on Hg atom at MRCI level.
Gleichmann and Hess (1994b)	LiHg. DK including SO. MRCI.
Kutzelnigg et al. (1994,1995)	Relativistic HF based on DPT.
Park and Almlöf (1994)	Pt_2, M_2, MH; M=Ag,Au. Test two-electron terms in DK (HF, MP2).
Sadlej and Snijders (1994)	Spin separation in the regular Hamiltonian approach. Cp. Dyall (1994a).
Shukla and Banerjee (1994)	A four-component relativistic DF method for valence electrons only. An effective core-valence potential constructed. Tested on atoms, Li-S.
van Leeuwen et al. (1994)	ZORA solutions for H-like atoms are scaled Dirac ones.
van Lenthe et al. (1994a)	Relativistic total energy using regular approximations. For Au_2, AuH, ZORA is close to frozen-core.
van Lenthe et al. (1994b,1996c)	Reviews on regular Hamiltonians.
Faas et al. (1995)	The ZORA formalism applied to the DF equation. Xe, Rn. The deep core densities can be improved by scaling.
Ottschofski and Kutzelnigg (1995)	DPT tested on atomic ground states of He-Rn.
Sadlej et al. (1995)	Four-component regular Hamiltonians.
van Lenthe et al. (1995)	Solves the 2nd-order Dirac equation for the large component in a Slater basis. Tests on U atom.
van Wüllen (1995)	DFT by DPT. Tests on $M(CO)_n$, MH; M=Ag,Au; Au_2.
Wolff et al. (1995)	Self-consistent SO and Zeeman terms in otherwise NR ab initio calculations. Magnetic structure factors for $CsCoCl_5$.
Hada et al. (1996)	^{183}W NMR shielding in WX_6; X=F,Cl, WO_4^{2-}. DK.
Hess et al. (1996)	A mean-field SO method ('AMFI') for correlated wavefunctions.
Kellö and Sadlej (1996a)	Basis sets for highly correlated DK calculations for Groups 11 and 12 (Au, Hg).
Kutzelnigg (1996)	Theory of stationary DPT (Direct Perturbation Theory) of relativistic corrections.
Molzberger and Schwarz (1996)	Effects of different order in α^2 on energies of H-like atoms. Compare Dirac with 1st- and 2nd-order DK.
Nasluzov and Rösch (1996)	DFT code within SR DK approximation with analytical energy gradients. Tested on Au_2,AuH,AuCl, $M(CO)_6$; M=Mo,W; $[M(PH_3)_2O_2]$; M=Pd,Pt.

Reference	Comments
Neogrády et al. (1996)	Polarized basis sets for high-level correlated calculations of electric properties. Polarizabilities for M,M^+; M=Cu-Au.
Rösch et al. (1996)	DK DFT molecular calculations. Review.
Rutkowski (1996)	Basic aspects of regular PT.
Rutkowski and Schwarz (1996)	Effective DPT Hamiltonian for near-degenerate states. Formalism.
Snijders and Sadlej (1996)	Perturbation versus variation treatment of regular relativistic Hamiltonians. Latter preferred.
van Lenthe (1996)	The ZORA equation. Thesis.
van Lenthe et al. (1996a)	Solve the Dirac equation using the FW transformation and large components only. Tests on U atom.
van Lenthe et al. (1996b)	SO effects in closed-shell molecules via ZORA. Tested on several diatomics containing I to Bi.
van Wüllen (1996b)	DFT with DPT. Tests on TM carbonyls.
Barysz (1997)	Compares Pauli PT, DPT and Dirac levels for H-like systems.
Barysz and Sadlej (1997)	Expectation values $\langle O \rangle$ in approximate two-component theories. Example $O = 1/r$.
Barysz et al. (1997)	Two- or one-component Hamiltonians to arbitrary order in α^2.
Boettger (1997)	SR LCGTO DK code tested on atoms. Ce, Au, Pb, Pu.
Dyall (1997); Dyall and Enevoldsen (1999)	'Normalized elimination of small components'. Can make light atoms non-relativistic (local α=0).
Fleig et al. (1997)	Use of time-reversal symmetry between Kramers pairs in MC DK calculations, especially CASSCF.
Franke (1997)	One-electron systems using DPT.
Geipel and Hess (1997)	DK approach for solids (in crystal HF). Ag, AgX; X=F-Br. Bond contraction. Metal stabilized, salts destabilized by relativity.
Havlas and Michl (1997)	SO effects in triplet tetramethyleneethane biradical.
Klopper (1997)	1st-order DPT relativistic corrections to correlated calculations.
Kutzelnigg (1997)	Relativistic 1-electron Hamiltonians 'for electrons only' and the variational treatment of the Dirac equation. Relations to 'regular approximation', DK and minimax principle.
Miadoková et al. (1997)	Standardized basis sets for highly correlated DK calculations of electric properties. IP of Li-Fr, Be-Ba. Polarizability of K-Fr, Li^+-Fr^+, Ca-Ba.
Ottschofski and Kutzelnigg (1997)	DPT tested on He-like systems. r_{12} wave functions. Z=1-120.
Philipsen et al. (1997)	CO adsorption on (111) surfaces of Ni,Pd,Pt. ZORA.
Rutkowski and Kozlowski (1997)	Relativistic H atom in static, uniform **B**. DPT.
Sjøvoll et al. (1997a)	PdH. SO CI at DK level or DF level.
Sjøvoll et al. (1997b)	Determinantal approach to SO CI.
Sundholm and Ottschowski (1997)	DPT incorporated into the atomic MCSCF code LUCAS. Tested on Zn-Hg, Ne-Rn.
van Lenthe et al. (1998)	ZORA calculations of molecular g-tensors.
Wahlgren et al. (1997)	SO splitting of the Tl atom. BP/DK.
Császár et al. (1998)	Relativistic corrections to potential energy surface and rovibrational levels of water.
Dyall (1998a)	Attempted search for a variational α^2 method.

Reference	Comments
Franke and van Wüllen (1998)	Comparisons of PT and DPT at MP2 level. He-Ar, MH; M=Cu-Au.
Gagliardi et al. (1998a)	A two-centre implementation of DK. The MAGIC code.
Havlas et al. (1998); Havlas and Michl (1998)	SO coupling in organic biradicals. Correlated ab initio calculations including the BP Hamiltonian. Carbenes and silylenes.
Kellö and Sadlej (1998a)	Picture-change effect on expectation values. DK and spin-free Pauli. EFG in HX; X=Cl-At as example.
H. Müller et al. (1998)	HF. Spectroscopic accuracy with CCSDT1-r_{12}. PT relativity.
Rutkowski et al. (1998)	DPT on H_2^+-like systems.
Sjøvoll et al. (1998a)	PtH. Include SO during CI or after CI stage.
Sjøvoll et al. (1998b)	New way to treat the p-dependent terms in DK calculations. Tests on Br_2.
van Lenthe et al. (1998)	Calculation of g-tensors and M1 hyperfine interactions at ZORA level. Exact relations between Dirac and ZORA for H-like atoms. Tests on TiF_3, 5- or 7-atom coinage-metal clusters.
van Wüllen (1998)	DFT with ZORA. Introduces a model potential for use in the kinetic-energy operator. Tests on MM', MX; M=Cu-Au, X=H,F,Cl.
Wahlgren et al. (1998)	Keep one-centre DK terms, only. Tests on Au_2, UO_2^{2+}.
Balinsky and Evans (1999ab)	Stability of one-electron molecules. 'No-pair' Hamiltonian.
Dyall and van Lenthe (1999)	An infinite-order relativistic approximation (cp. ZORA).
Griesemer and Tix (1999)	Claims that the N-electron no-pair model is magnetically instable for all values of α.
Havlas and Michl (1999)	Zero-field and SO splittings in triplets of m-xylylene.
Kutzelnigg (1999a)	Effective Hamiltonians for degenerate and quasidegenerate DPT. Relationship to FW transformation.
Kutzelnigg (1999b)	Relativistic corrections to magnetic properties. DPT.
La Cour Jansen et al. (1999)	Evaluation of SO matrix elements in a spin-adapted basis.
J. M. L. Martin and de Oliveira (1999)	Atomization energies of many 1st-row -to- 3rd-row (H-Cl) molecules. PT relativity.
J. M. L. Martin and Taylor (1999)	Atomization energy of SiF_4. PT relativity.
Miadoková et al. (1999)	MF; M=K-Fr. Electric properties. PT/DK.
Nakajima and Hirao (1999)	'RESC' scheme: eliminate small components, use $T = \sqrt{p^2c^2 + m^2c^4} - m$ kinetic energy. Tests on Ag, Au, AgH, AuH.
Nakajima et al. (1999)	Combine DFT and RESC. Tests on MH,MX; M=Ag,Au.
Rutkowski (1999)	Iterative solution of one-electron DPT equations.
Schwerdtfeger et al. (1999)	EFG in HCl and CuCl. Accuracy of the DFT approach. DK.
Tatchen and Marian (1999)	Test approximate SO Hamiltonians on NC_nH^+; N=4,5, NC_4N^+. AMFI approximation excellent.
van Lenthe et al. (1999)	Analytical energy gradients for geometry optimization using ZORA. Tests on W, Os and Pt carbonyls.
Visscher and van Lenthe (1999)	Separation between SR and SO effects done in three different ways with three different results. U^{91+}.
Wolff et al. (1999)	NMR shifts using ZORA and DFT. ^{199}Hg in LHgL'.

Table 7.4: Methodological density-functional theory papers.

Reference	Comments
W. F. Schneider et al. (1991)	DV DFT studies of 3-coordinate An complexes. Review.
L. Yang et al. (1993)	Fully numerical (FEM), fully relativistic DS for light diatomics, LiH, Li_2, BH, C_2.
Bastug (1994)	Accurate DS total energies for molecules.
Onoe et al. (1994ab); Onoe (1997)	Analyses relativistic effects on DVM-DFT MO:s for Cu_2, AuH, Pb_2, XF_6;X=S-Po, Mo-W,Re→Pt, U,Np,Pu.
Schreckenbach et al. (1995)	Implementation of analytical energy gradients in SR DFT methods. Tests on $M(CO)_5$; M=Fe-Os, $M(CO)_6$; M=Cr-Mo.
Hirata (1996)	Applications of DS-DVM in actinide chemistry.
Malkin et al. (1996)	NMR shieldings including SO.
Mayer et al. (1996)	M_2; M=Cu-Au, AuH, AuCl. Various functionals, finite nucleus effects studied.
Nasluzov and Rösch (1996)	DFT code within SR DK approximation with analytical energy gradients. Tested on Au_2,AuH,AuCl, $M(CO)_6$; M=Mo,W; $[M(PH_3)_2O_2]$; M=Pd,Pt.
van Wüllen (1996a)	Can the common PP be used in DFT? Compared with AE. A: Yes.
Baerends and Gritsenko (1997)	DFT on molecules reviewed.
Fricke et al. (1997)	Review on the DFT DVM applications on superheavy elements.
Menchi and Bosin (1997)	DFT PP in QMC.
Malkina et al. (1998)	NMR shieldings including SO using AMFI.
Schreckenbach and Ziegler (1998)	DFT calculation of NMR shifts and ESR g-tensors. Review.
Ellis and Guenzburger (1999)	Review on the DFT DVM.
Schreckenbach et al. (1999)	DFT calculations on actinide compounds.
van Wüllen (1999)	Status of all-electron DFT on molecules.
Varga et al. (1999)	Latest description of the DV DFT methods. Tests on M_2; M=Cu-Au.

Table 7.5: Relativistic or quasirelativistic scattered-wave (multiple-scattering) calculations.

Reference	Comments
Parsons and Till (1993)	Introduction of non-muffin-tin corrections permits bond-length optimizations. Octahedral MF_6; M=Mo,W,U.
Vijayakumar and Gopinathan (1993)	SW method with the authors' Ξ functional. Tests on PES of SF_6, MnO_4^-.
Subramanian and Ramasami (1995)	MX_4; M=Zr,Hf; X=Br,I. PES. Adjustment of spheres discussed.

The next Table 7.6 contains reviews and methodological papers on relativistic or quasirelativistic pseudopotential (effective core potential) calculations. See also Table 4.8.

Table 7.6: Pseudopotential (effective core potential) methods.

Reference	Comments
Vijayakumar et al. (1993)	An efficient, relativistic MRCI method. Tests on Pb_2, Bi_2.
Schwerdtfeger et al. (1995a)	Accuracy of the PP approach tested on InCl, $InCl_3$. Small core better.
Sekkat et al. (1995)	Effective potentials for *molecular* EH_3 groups, E=N-As. Tested on AH_3-EH_3, A=B-Tl.

Reference	Comments
Seijo and Barandiarán (1996)	Use of embedded cluster models, based on PP in study of laser materials. M:M'O; M=Sc→Zn; M=Mg-Sr. Tl^+:$KMgF_3$.
Titov (1996)	A two-step PP method proposed. Restores the core-region orbitals for hfs properties or PNC applications.
Menchi and Bosin (1997)	DFT PP in QMC.
Schimmelpfennig et al. (1998ab)	The 'atomic-mean-field integral (AMFI)' approach to SO CI.
Skylaris et al. (1998)	Efficient method for PP integrals. Uses projection operators. Part of the MAGIC code.
Balasubramanian (1998)	ECP techniques for heavy-atom molecules.
Takahashi et al. (1999)	SCF method with SO. D_{2h} or subgroups.
Yabushita et al. (1999)	SO CI using graphical unitary group approach. Implementation with PP SO operators. COLUMBUS package.

Table 7.7: Semiempirical methods.

Reference	Comments
Christoffersen and Hall (1966)	Orbit-orbit coupling in aromatic molecules. Effect on magnetic susceptibility of benzene.
Minaev (1983)	SO effects in molecular spectroscopy and chemical kinetics.
Bengtsson and Hoffmann (1993)	Pb_2X^{3+} structural units; X=F-I. Pb...Pb discussed.
Breza (1993ab,1994)	Cluster models for Y-Ba-Cu-O superconductors. CNDO/1.
A. Datta et al. (1993)	Cluster models for $YBa_2Cu_3O_7$. REX.
Garcia et al. (1993)	Model electron-hopping hamiltonian for IP of Rg_n, Hg_n.
Milletti (1993)	$M_2X_4(PH_3)_4$; M=Mo,W; X=Cl,Br. Fenske-Hall. Influence of halide ligands on M-M quadruple bond.
Reindl and Pastor (1993)	Pb_n^{2+}.
von Grünberg et al. (1993)	Using DIM for semiempirical band structures. Ar-Xe crystals.
Boča (1994)	$[Au(Pt\text{-}Bu_3)_4]^{2+}$ bonding. CNDO/1. Various phosphines compared.
Boča et al. (1994)	Cu(II) dimethylpyrazole complexes. INDO/1.
Burdett et al. (1994)	Au...Au interactions in $X_nA(AuPR_3)_m$ molecules.
Calhorda and Veiros (1994)	Au(I)...Au(I) interactions. Chains, rings. EHT.
Cory et al. (1994)	INDO approach for actinide compounds. AnX_n; n=4,6; An=Th-Pu. $An(COT)_2$, amide/imide complexes.
Dionne and Allen (1994)	Bi-O-Fe hybridization for magneto-optical states in $Y_{3-x}Bi_xFe_5O_{12}$.
Lawrence and Apkarian (1994)	SO states of I atoms in crystalline Kr and Xe.
Turi Nagy et al. (1994)	A SR INDO approach. Tested on tetrahedral XY_4 molecules.
Akamova et al. (1995)	MNDO on linear clusters of Hg_n, n=2-4.
Boudreaux and Baxter (1995); Boudreaux and Baxter (1997)	$Sm(Cp^*)_n^{q+}$ systems.
Braun et al. (1995); Braun et al. (1996)	$[Th_{12}N_6Cl_{41}]$ clusters. EHT.
Z.-C. Dong and Corbett (1995)	Tl_n; n=12,13 models for Zintl compounds. REX/EHT.
Endo et al. (1995)	Si and C NMR shifts in SiX_4, $CH_{4-n}X_n$; X=Cl-I; n=1-4. PM3+SO.

Reference	Comments
Estiú et al. (1995)	Ln bis(octaethylporphyrinate); Ln=Ce,Eu. INDO-S/CI.
Watkins and Williams (1995)	Semiempirical model for substitutional impurities Ni^-, Pd^-, Pt^- and Au^0 in Si. g-tensor.
Boča (1996)	$[Pt(CO)(AuPPh_3)_8]^{2+}$. CNDO/1.
Böckmann et al. (1996)	SO coupling in organic molecules. MNDOC-CI. Triplet-state reactivity.
Braun and Simon (1996)	Octahedral $Th_6H_xBr_{15}$ clusters, x=5,7. EHT band structure with parameters of Pyykkö et al. (1989).
Breza (1996)	Cluster models for La-Ba-Cu-O superconductors.
Hammer et al. (1996)	CO on M(111); M=Ni,Cu,Pd,Ag,Pt,Au; Ru(0001),Cu_3Pt. Simple model for d-band hybridization proposed.
Kane et al. (1996)	PbS nanoclusters. Up to 912 atoms. SO included.
Michl (1996)	SO coupling in biradicals. 2-electron-2-orbital model.
Thiel and Voityuk (1996)	Extension of MNDO to d orbitals. Cl-I, Zn-Hg. Tested on heats of formation of a 575 molecule set.
Belkhiri et al. (1997)	UF_5, AnO_2^{n+}, An=Th-Am. Rel. effects on bond angles.
Calhorda et al. (1997)	Au(I)...Au(III) interactions. EHT.
J. A. González et al. (1997)	NMR ^1J coupling constants in Me_3XY; X=C-Pb; Y=F,Cl. MNDO-level correlated approach.
Muinasmaa et al. (1997)	Carboxylic acid complexes of M^{2+}; M=Mg,Zn,Cd,Pb. PM3.
Sasaki et al. (1997)	SO-induced electron-spin polarization in donor-acceptor complexes containing heavy halogen atoms. ESR.
D. P. Huang and Corbett (1998)	$TaAs_4^{7-}$ and $(TaAs_4Tl_2)^{5-}$ clusters. EHT.
Julg (1998)	Absorption spectra of Pb^+ and Pb^{3+} in amazonite, KSi_3AlO_8. $6s \rightarrow 6p$ handled with simple MO model.
Lobayan and Aucar (1998ab)	NMR spin-spin coupling constants within PM3 parametrization, CLOPPA scheme. As-Bi, Ga-Tl, Si-Pb.
Minaev and Ågren (1998)	SO coupling in oxygen-containing diradicals. Reaction paths. MNDO CI.
Naumkin (1998)	DIM model for Rg·X_2 systems. Ar·I_2 potential.
Neese and Solomon (1998)	INDO/S-CI for ZFS and g-factors in TM complexes. $FeCl_4^-$ as example. Results compared with BP PT ab initio ones.
Omary and Patterson (1998)	$[Ag(CN)_2]_3$ chain model for solid $Tl[Ag(CN)_2]$. EHT.
W.-J. Li et al. (1999b)	Introduce CI to A. J. Stone's (1963)[2777] theory of the g-matrix. Applications on $[MOX_n]^{m-}$; M=V,Cr,Mo; X=F-Br. INDO.
Olenev et al. (1999)	$(P_2Hg_6)^{8+}$ model for solid Hg_2PCl_2. EHT.
Seo and Hoffmann (1999)	Structures of solid elements P-Bi. EHT.
Seong and Anderson (1996)	Water dissociation on Pt anodes. Semiempirical model.

Table 7.8: Relativistic crystal-field theory.

Reference	Comments
Richter et al. (1992,1995)	Crystal-field parameters of $SmCo_5$ obtained from a solid-state ab initio calculation.
Burdick et al. (1993)	Correlation effects on two-photon absorption intensities for Eu^{2+}.
Burdick and Reid (1993)	Dito for Gd^{3+} in LaF_3.
Chatterjee and Buckmaster (1993ab)	Relativistic crystal field theory.
Hubert et al. (1993)	Eu^{3+} and Am^{3+} in cubic-symmetry site of ThO_2.
Lulek (1993)	SO coupling for f electrons in a crystal field.
Parrot and Boulanger (1993, 1997)	SO for d^5 ions in crystals.

Reference	Comments
Bonča and Gubernatis (1994)	QMC for magnetic impurity with SO and crystal-field splitting. Single-impurity Anderson model.
Steinbeck et al. (1994)	Obtain crystal-field parameters for the $4f$ states of Er and Dy in Ag or Au from solid-state DFT calculations.
Kornienko et al. (1995)	Effect of CI on SO parameter of Ln ions.
Schamps et al. (1995)	LaO. Ligand field model tested against PP MRCI.
Dushin et al. (1996)	Crystal-field theory for trivalent Er, U, Md.
Steinbeck et al. (1996)	Obtain crystal-field parameters for the $4f$ states of Sm in Fe and Co intermetallics from solid-state DFT calculations.
Bencheikh and Schamps (1997)	Relativistic ligand field theory. SO in diatomics.
Brooks et al. (1997)	Crystal field excitations of Ln are combined from $4f$ excitations and a cloud of shielding conduction electrons. Spin Hamiltonians of TmSb and PrSb reproduced *ab initio*.
D.-D. Dai et al. (1998)	Crystal-field parameters from DFT for diatomic CeO, CeF.
S. Edvardsson and Klintenberg (1998)	Shielding parameters for crystal-field theory from DF atomic calculations.
Rahman (1998)	Crystal-field excitations in UO_2.
Ren et al. (1998)	LnF; Ln=Pr→Yb. Low-lying levels.
Smentek (1998)	Spectroscopy of Ln ions in crystals.
Smentek and Hess (1998)	Odd-rank crystal-field parameters. Determine intensities. Are related to each other.
Zhorin and Liu (1998)	f-elements in $LaCl_3$.
Smentek (1999)	Relativistic contributions to E1 transitions of Ln ions in crystals. SO part.

Table 7.9: Relativistic theories of molecular properties.

Reference	Comments
Ågren and Vahtras (1993)	SO coupling in molecular Auger spectra. Water.
Aucar and Oddershede (1993)	Nuclear spin-spin coupling in Polarized Propagator approach.
Pegarkov (1993)	Adiabatic states of diatomic molecules with large SO coupling.
Zhu et al. (1993)	SO and rotational autoionization in HCl and DCl.
Dubernet and Hutson (1994)	Atom-molecule van der Waals complexes for open-shell atoms. Different angular-momentum coupling cases (cp. Hund's cases).
Serebrennikov and Steiner (1994); Steiner and Serebrennikov (1994)	Theory of spin-rotational relaxation for electrons with $S^{\text{eff}} = \frac{1}{2}$. 'Adiabatic rotation of effective spin'.
Ågren et al. (1996)	SO effects in molecules.
Ballard et al. (1996)	Proton NMR shifts in HX; X=F-I. 'No-pair' + SO.
Fukui et al. (1996)	Relativistic effects in NMR shielding. Lowest order.
Fukui and Baba (1998)	NMR shielding at no-pair level.
Kaupp et al. (1998b)	A simple interpretation for SO-induced NMR shifts, analogous to FC spin-spin coupling. Applied on iodo-organic compounds. ^1H and ^{13}C shifts.
Aucar et al. (1999)	'Diamagnetic' (A^2) term for magnetic properties in Dirac theory.
Baba and Fukui (1999)	Gauge-origin-independent relativistic effects in NMR shifts.

The following Table 7.10 contains production results for molecules, classified by the heaviest element, or group of elements in them. The methods of calculation are explained in Table 10.1 in the Appendix. The last column gives the way of including relativistic effects. For series of chemical elements, a hyphen, '-', goes down a column and an arrow, →, from left to right in the Periodic Table.

Table 7.10: Production results for molecules.

Element		Compounds	Ref.	Method
1	H	H_2, H_3^+.	9423	DPT
		Accurate relativistic corrections for H_2^+, H_2.	7140	PT
		Accurate relativistic corrections for H_3^+. Rovibrational analysis given.	7141,8166	PT
		H_2 ground state. $R \leq 12$ au.	10223	PT
		H_2 excited states.	10224,10225	PT
		H_2 ground state. 2D FEM. DF/HF.	10268	DF
2	He	Spin-orbit and spin-spin coupling in He_2, He_2^-.	6960	PT
3	Li	DF/HF comparisons for Li compounds.	7398	
		LiH, Li_2. DS/HFS.	10268	DFT
4	Be	Be_2. Explicitly correlated. Rel. D_e decrease -0.56%	7816	PT
		Be_2. Rel. D_e decrease -0.42%	8831	PT
5	B	BH. DS/HFS.	10268	DFT
		BF. BF_3, whose atomization energy reduced by 0.7 kcal/mol.	6865	DK
6	C	C_2. DS/HFS.	10268	DFT
		C_{60}^{x+}, x=0-7	6851	DFT
7	N	N_2. Phosphorescent A $^3\Sigma_u^+ \rightarrow$ X $^1\Sigma_g^+$ decay, Vegard-Kaplan band.	9092	PT
		NH^+ FS.	9148	PT.
8	O	O^+-O collisions.	8019	PT
		O_2^{2+} predissociation.	7567	PT
		O_2^+, O_2^-. FS splitting. Up to CCSD(T) level.	10126	DF+corr.
		CO $V(R)$	6815	PT
		OH. SO splitting. NO^+ radiative lifetime. H_2O^+ Renner-Teller effect.	6873	PT
		H_2O. Rovibrational levels. CCSD(T), QZ.	7307	PT
		H_2O.	9333	DFB
		HCO SO coupling.	9188	PT
9	F	HF. R/NR.	8833	PT
		HF. PT relativity, CCSDT1-r_{12}.	8994	PT
		BF. BF_3, whose atomization energy reduced by 0.7 kcal/mol.	6865	DK
		FO. FS splitting. Up to CCSD(T) level.	10126	
		C_2F_4	6867	DK
		CF_3, CF_4, C_2F_4, :$CFCF_3$, Heat of formation.	7468	PT
		SO corrections to F+D_2→DF+D.	8048	PT
10	Ne	H^++Ne high-energy collision.	8500	DFT
		BNe. Lifetime of C $^2\Delta$. MRCI.	9793	PT
13	Al	AlF,AlCl. EFG, Q(Al) derived.	8334	DK
		AlH_2, AlAr.	9170	DF+CCSD(T)
		AlNe. SO. CCSD(T).	10271	PT
		AlX_4^-; X=H,F-I. ^{27}Al NMR shifts.	9022	PT

Element		Compounds	Ref.	Method
14	Si	SiH_4. Heats of formation in Si chemistry.	7258	DK
		SiH_4.	8401	DPT
		SiF, SiF^+. Accurate D_0.	9393	PT
		SiF_4 atomization energy.	8834	PT
15	P	PH_n, PH_n^+; n=1-3	6788	PP
		PO_n, PO_nH; n=1-3	6862	DK
16	S	S_n^q; n=2,3; q=0,-1.	7988	NR+SO
		SH ($A\ ^2\Sigma^+$). Fragmentation. SO.	9387	PT
		SO, SO_2. Atomization energies.	6866	PT
		Adsorbed sulfur oxide anions.	9090	
17	Cl	HCl 2p PES interpreted.	7615,7695	DF+CI
			7696	
		ClO. FS splitting. Up to CCSD(T) level.	10126	
		$H+Cl_2 \rightarrow HCl+Cl$. $Cl+HCl \rightarrow ClH+Cl$.	10121	MP2:
		Rel. effects on reaction energy.		R/DK/NR
18	Ar	Ar_2^+, Ar_3^+.	7797	PP
		BAr. External heavy-atom effect by Ar on the SO. MRCI.	9792	PT
		AlAr.	9170	DF+CCSD(T)
		GaAr, $GaAr^+$.	9160	PP,PT
		MAr^+; M=Fe,Co,Ni,Cu,Zn; Ar = argon	6853	DFT
		Ar^{8+}–C_{60} collision system.	9968	DFT
		$Ar \cdot I_2$ ground-state potential. Linear and T.	8496	DK
		DF-level thermochemistry for Pople's G2/97 test set of		
		148 species, up to Ar (Z=18. Atomization energies.	8311	DPT
19	K	KF, KCl. EFG, Q(K) derived.	8328	DK
		NaK. Photodissociation.	9388	PT
20	Ca	$CaCl^{2+}$.	10227	PP
		CaX^{2+}, X=Br, I.	6645	PP
21	Sc	ScN.	7377	PP
22	Ti	TiF^{n+}; n=1-3.	9618	PP
		TiCl, TiH, TiH^+.	6861	DK
		TiF_3.	6896	DFT
		$H_2Ti(\mu\text{-}H)_2TiH_2$. SO.	10190	PT
24	Cr	Cr_2.	6673,6675	PT
			9430	PT
		Cr_2.	9838	PP
		$Cr_2(O_2CH)_4$.	6674	PT
26	Fe	$FeO^+ + H_2$.	7376	PT
		FeL^+; L=Xe,CO_2,N_2,CH_4.	7457	PP
		Fe^+ + small alkanes.	8006	DFT
		FeCO, FeL^+; L=CO,H_2O,CH_4.	9395	PT
		$Mn^{2+/3+}$ and $Fe^{2+/3+}$ (aq) redox potentials and pK_a^J.	8614	DFT
		$[FeHgCp_2]^{2+}$, $[FeCp(C_5H_4)Hg]^+$ ferrocene derivatives.	8870	DFT
27	Co	CoH, CoH^-	7748	DK
		$HCo(CO)_4$. SO-induced radiationless transitions.	7997,9390	PT
28	Ni	Ni^{2+}:MgO. Electronic spectrum.	8703	PP
		Ni_2^+: symmetry breaking	8890	PT
		NiH_2	6835	PT
		MH^+, MCH_3^+, MCH_2^+, M = Sc→Ni.	6972	PT

Element		Compounds	Ref.	Method
		NiC. Low-lying states. X $^1\Sigma^+$.	9729	PT
		$Ni(C_2H_4$ + ferrocene.	9245	PT
		$M(CO)_x$; M=Cr,Fe,Ni.	9208	PT
		Octahedral Ni(II).	9389	PT
		NiF_6^{4-}. Zero-field splitting.	9392	PT
29	Cu	Cu_2, Cu_2^+, CuH, CuF, CuCl.	8761	PP
		Cu_3, X $^2E'$, SO included. Geometric phase.	8421	PT
		M_2, MH; M=Ni,Cu.	9288	PT
		CuH.	8401	DPT
		CuCl. Low-lying excited states.	9804	PT
		CuX; X=Cl-I. Low-lying excited states.	9805	PT, DF+CI
		CuX; X=F-I. Lifetimes of excited $^1\Sigma$ states.	9357	PP
		CuF. EFG. CCSD(T).	9191	DF, DK
		CuX, Cu_2X; X=O-Po.	8762	PP
		AlCu.	6863	PT
		CuM, Cu_2M, CuM_2; M=Si-Sn.	9263	PP
		$[MO_2]^{3-}$; M=Fe→Cu in A_3MO_2 crystal field.	10167	DFT
		$(Cu_2S)_n(PR_3)_m$.	7411	PP
		$(Cu_2Se)_n$, $(Cu_2Se)_n(PR_3)_m$.	7412,9581-9583	PP
		Cluster models for $Cu_2O(100)$. H_2O adsorption.	9079	PT
		Cu + CH_2N_2.	7311	PP
		CO_2 + $CuH(PH_3)_2$.	9536	PP
		$L_n(Cu_2O_2)L_n$ oxyhemocyanin models, L=NH_3,PH_3.	8697	DFT+PP
		Models of blue copper proteins. CASPT2.	9243,9244	PT
		Test case $Cu(NH_3)_2(SH)(SH_2)^+$. Level shifts $\leq$ 1%.	7339	PP
30	Zn	Zn_2.	8164	PP
		ZnH.	7878	PP
		ZnH^+, ZnH_2, Zn_2H, HZnZnH, H_2Zn_2, H_4Zn_2.	10168	DFT
		MX_2; X=F,Cl; M=Ca→Zn.	6853	DFT
		MAr^+; M=Fe,Co,Ni,Cu,Zn; Ar = argon	9160	PP,PT
31	Ga	GaAr, $GaAr^+$.	7675	PP
		Ga_2P_2	7677	PP
		Ga_2P, GaP_2, their ions	7678	PP
		Ga_3P_2, Ga_2P_3	7681	PP
		Ga_3P, GaP_3	9189	PP
		GaF. Q(Ga) obtained.	6858	DK, DF+CCSD
		GaX_n; X=F,Cl; n=1-3. SR corr.	7286	PT, DK
		R_2Ga-GaR_2.	7357	PP
32	Ge	Ge_5.	9394	PP
		GeH_n; n=1-4, Ge_2H_n; n=1-6. Heat of formation.	7368	PT
		$GeCl^+$.	8631	PP
		GeCl.	8632	PP
		GeF.	10241	PP
		GeF^+.	8329	PP
		GeO, GeS. EFG, Q(Ge) derived.	8149	DK
		$GeCH^+$.	9530	PP+DFT
33	As	As_2, As_2^+.	6643	PP
		AsH.		

Element		Compounds	Ref.	Method
		AsF.	8655	PP
		AsX_2, AsX_2^+, X = Cl, Br.	8574	PP
		As speciation in minerals and aqueous solution.	10002	PP
		EH_3 effective potential, E=N-As.	9659	PP
		$GaAs_2$, Ga_2As.	6724	MS
		Ga_2As_3.	6718	MS
		Ga_3As_2, Ga_2As_3.	8646	PP
34	Se	$Se_n^{0/-1}$; n=2,3.	7989	PP
		Me_2SeX_2; X=F-At.	8252	DFT
		$ClSeNSeCl^+$, a new cation.	7063	PP
		$(Cu_2Se)_n$, $(Cu_2Se)_n(PR_3)_m$.	7412,9581-9583	PP
		Selenoiminoquinones: Se ... O interaction.	6820	PP
35	Br	Br_2. Lowest levels, tests new DK method.	9769	DK
		HBr.	9681	PP
		$CaBr^{2+}$.	6645	PP
		AsH^+, SeH, HBr^+, BrO, BrF^+, $NaBr^+$, Br_2^+. SO splittings.	6963	PP
		BrCl. EFG.	7741	DK
		BrO_3.	9140	PP
		PH_2Br.	7052	PP
		2nd-order SO for GeH_4, ... Br_2.	6963	PP
		Ni-Br collision. Very short R.	8503	DFT
		$C_2H_4 \cdot\cdot X^-$, halopyridines; X=F-Br. Heavy-atom effects on phosphorescence using AMFI SO.	9496	PT
36	Kr	KrF, KrF^+, KrF_2.	8036	PP
37	Rb	RbF, RbCl. EFG, Q(Rb) derived.	8330	DK
		MM'; M,M'=Li-Rb. Electric properties.	10053	PT
38	Sr	Sr_2.	7032	PP
		$SrAr^+$.	10238	PP
		SrF. RI-MP2.	10192	PP
		MO, OMO, MO_2; M=Be-Sr.	6677	PP
		L→Sr^{2+}; L = [R_3P=O], amides, pyridine.	6921	PP
		OPR_3 complexes of Sr^{2+}, $Sr(NO_3)_2$. R=H,Me,Ph.	8085	PP
39	Y	Y_n, n=1-4.	7354	PP
		YC_n; n=2-6.	9450,9451	PP
		$MY_6I_{12}^{2-}$; M=Ru,Os.	6715,6716	MS
40	Zr	Zr_3.	7353	PP
		Zr_5.	8767	PP
		ZrF^{n+}; n=1-3.	9618	PP
		MCl; M=Ti,Zr. Ground states $^4\Phi$, $^2\Delta$, respectively.	9532	PP
		Zr_2 + ethene, butadiene. Diels-Alder.	9448	PP
		ZrI_4, $Zr(TeSiH_3)_4$.	8248	DV DFT
		ZrX_6^{2-}; X=F-I.	7922,9343	PP
		MO; M=Ti,Zr. IP.	8714	DFT
		Bridge bonding of N_2 to M_2 systems, M=Ti,Y,Zr.	6970	PT
		ZrN_2-L complexes.	6847	PP
		Cp_2MR^+; M=Zr. Ziegler-Natta catalysis.	8797	DFT
		$Cp_2ZrCH_3^+$ as model polymerization catalyst.	7777	PP
		Ethylene polymerization catalyzed by M-chelating	9002	PP

Element		Compounds	Ref.	Method
		alkoxide; M=Ti, Zr.		
		$(p2n2)Zr(\mu-\eta^2\text{-}N_2)Zr(p2n2) + H_2$. $(p2n2)=(PH_3)_2(NH_2)_2$	6846	PP
		$(NH_2)_2M{=}NH$; M=Ti,Zr CH_4 adducts	7312	PP
		$Cl_2Zr{=}E$; $E=MH_2$ (M=C-Sn), MH (M=N-Sb), M (M=O-Te)	6910	PP
		$Zr(OH)_2(H_2O)_2Cl_2$. Distortion from C_{2v} intrinsic.	7656	PP+DFT
		$L_nZr{=}NX + CH_4$	7318	PP
		$Zr@C_{28}$	7077	PP
41	Nb	Nb_n; n=8-10	7898	PP
		Nb_3O, Nb_3O^+.	10265	DFT
		NbN	7719	PP
		MO, MO_2, MO_2^+; M=Ti,V,Zr,Nb. Reactions with C_2H_4, C_2H_6	7967	PP
		NbO. IP.	8714	DFT
		NbCO	9932	PP
		$NbCl_5$	7868	DK
		Nb_4C_4, Nb_5C_6, Nb_6C_7	7103	PP
		$[Cp_2NbH_3]$ + Lewis acid A;	7111,7112	PP
		A = $HBO_2C_2H_2$, BF_3, BH_3. H_2 elimination		
		$Nb_n^+ + C_6H_6$; n=1,2.	9460	PP
42	Mo	$MoCl_5$	7644	PP
		MoC. Low-lying states.	9728	PT
		MoC_4	8611	PP
		MCO, MCS; M=Y-Mo	8191	PP
		MoO. IP.	8714	DFT
		MoX_n^+; X=O,S; n=1-3.	8477	PT
		Mo_2 + ethene, butadiene. Diels-Alder.	9446	PP
		$M_n + N_2$; M=Nb, Mo; n=1-4.	6916	DFT
		Solid MoO_3. Adsorption of CO, H_2O on (100) surface.	9153	PP
		M_8C_{12}; M=Y→Mo.	8662	PP
		$Mo_2Cl_4(PH_3)_4$.	8702	DFT+PP
		$MMo(O_2CH)_4$;M=Cr,Mo. $Mo_2X_4(PH_3)_4$; X=Cl-I.	9757	PP
		MoO_4^{2-}, MoS_4^{2-}, $MoOCl_4$.	9758,9759	PP
		$M(CO)_6$; M=Cr-W. $M(CO)_5L$; $L=N_2,CS,NO^+$. DFT by DPT. For comments on the method, see.[10076]	10083,10084	DFT
		$M(CO)_6$; M=Cr,Mo.	10084	PP
		MoO_2X_2; X=F-I.	9998	PP
		H/D exchange in $CpMoH_3(PMe_3)_2$.	6583	PP
		$Mo_2Cl_4(PH_3)_4$ models for diphosphine complexes.	7428,7429	PP+DFT
		$[Mo_2Cl_4(PH_3)_4]$.	8174	PP
		$L_4Mo\overset{4}{=\!=}MoL_4$; $L=PH_3$,Cl.Mo-Mo quadruple bond. MCSCF required. UV, PES interpreted.	6964	PP
		$Mo(VI)H_4O + PH_3$, $Mo(VI)H_2O_2 + PH_3$.	9246	PP
		$(NH_3)_2(SH)_2Mo(VI)O_2 + H_2O$.	9247	PP
		^{95}Mo chemical shifts.	7078,7079	DFT
		CpMXY, CpMXYZ; M=Co,Ru,Rh,Mo; X,Y,Z=Cl,Me, NO,CO. Functionals compared.	8873	DFT
		Bispentalene dimolybdenum, $Mo_2(C_8H_6)_2$. Mo-Mo 234 pm.	7248	DFT
		$MO_2X_2 + CH_3OH$→$MX_2(OH)_2+CH_2O$. M=Cr,Mo;X=Cl.	7435	DFT+PT
43	Tc	$TcX(NR)_3$	6908	PP
		$[TcYX_4]^q$; Y=N,O; X=Cl,Br. Opt. transitions	6795	DFT

Element	Compounds	Ref.	Method
	$M_2(O_2CH)_4$, $M_2Cl_4(PH_3)_4$; M=Nb→Tc	7287	PP
44 Ru	RuN	9351	PP
	$[RuO_4]^{n-}$, n=0-2. Ground state for n = 2?	7408	DFT
	RuCO	9935	PP
	$M(CO)_5$; M=Fe,Ru	10084	PP
	$Y_2(PX_3)_2Ru{=}CZ_2$ alkylidenes; X,Y,Z=H,Me,F-Cl.	6909	PP
	MAr_n^+; M=Nb,Rh; n=4,6. Ar = argon	6929	PP
	$[Ru(NH_3)_6]^{2+/3+}$ redox pair	7060	PP
	$RuHX(CO)(PR_3)_2$; X=F-I, OH, OPh, SPh,...	9289	PP
	$Ru(H)_2(CO)_4$. Classical dihydride.	8577	DFT+PP
	Ru silylenes $(Cp)L_2Ru{=}SiX_2^+$	6708	DFT,PP
	$[Ru(P\text{-}P)_2"H_3"]^+$, P-P = diphosphine ligand	8842	PP
	$[Ru(bpy)_3]^{2+}$, bpy=bipyridine.	7402	DFT
	Cp_2M; M=Mn→Ni, Ru. Hyperpolarizabilities.	8856	DFT
	Cp_2M; M=V...Ru.	8869	DFT
	$Cp_2Ru_2(\mu\text{-}H)_4$. Anal. 2nd derivatives.	7311	PP
	$[Ru(H\cdots H)Cp(H_2PCH_2PH_2)]^+$. Nuclear dynamics.	7823	PP
	$LRh"H_4"$; L=Cp,Tp.	7824	PP
	Fluxional $TpRu(PPh_3)"H_2SiR_3"$ complexes. Tp=Hydridotris(pyrazolyl)borate.	9055	PP
	$Ru(CO)(PH_3)_2$ + benzaldehyde.	8852	PP
	$MO_2X_2 + CH_3OH{\rightarrow}MX_2(OH)_2{+}CH_2O$. M=Ru;X=O.	7435	DFT+PT
45 Rh	Rh_4.	7358	PP
	Rh_5.	8765	PP
	Rh_n^+, n=3-5.	8769	PP
	RhC.	9934	PP
	RhN. Low-lying states.	9730	PT
	$RhCO^q$; q=-1,0,+1.	10349	DFT+PP
	$RhCl_6^{3-}$	9391	PP
	$Rh_2 + H_2$.	7134	PP
	Rh_3 + CO.	8766	PP
	$Rh^{0/+/-}$ + CO, $+N_2$.	7655,8874	PP
	$Rh^+ + CH_4$.	10202	PP
	Butadiene + Rh_n; n=1,2.	7365	PP
	$CH_4 + Rh_n$.	6745	DFT
	Benzene + Rh^+, Rh_2^+.	8771	PP
	Rh alkene complex NMR shifts, UV spectra. CASSCF.	6614	PT
	$CpRhCO + CH_4$.	9802	PP
	$Cp^*Rh(PMe_3)$ + thiophene.	9569	DFT+PP
	$CO_2 + [RhH_2(PH_3)_3]^+$ or $RhH(PH_3)_3$	9536	PP
	$RhXL + CH_4$	7627	PP,DFT/MR-CI
	$[HRh(CO)_4]$ +CO $+H_2$.	9240	PP
	$[RhCl(CO)_3]_2$. $d^8 - d^8$.	9073	PP
	$[CpRh(C_2H_4)(\eta^2\text{-}C_2H_5)]^+$. H exchange.	8663	PP
	$[[Rh_2Cp_2(\mu\text{-}CH_2)_2]_2(\mu\text{-}S_4)]^{2+}$.	8878	PP
	$M_2(HNCHNH)_4$, $M_2(HNNNH)_4$; M=Nb →Rh.	7287	PP
	$RhCl(PH_3)_2$ as activator of SiH, SiSi and CH bonds.	8415	PP
	$[Rh(PH_3)_2]^+$ complexes of N-alkenylamides.	8394	PP
	$Rh(CO)_2^-$, $Rh(CO)_2F_2^{3-}$.	8746	PP

Element	Compounds	Ref.	Method
	$Rh_6(CO)_{16}$.	8284	PP
46 Pd	Pd_2.	9019	DFT+PP
	Pd_n; n=2,4. R/NR	10239	DFT
	Pd_5.	7362	PP
	Pd_n; n=1-6.	10062	PP
	Pd_n; n=1-6 + S, Cl.	10063	PP
	Pd_n; n=1-6. Ethylene adsorption.	7646	DFT
	Pd_n; $n \leq 147$.	8482	DFT
	PdH.	7714	DK
	PdH.	9768	DK/DF+CI
	MO, MCH_2; M=Y→Pd.	9742	PT
	MO_n; n=1-4; M=Y→Pd.	9743	PT
	MH, MO; M=Ni,Pd.	10154	PP
	PdC.	9931	PP
	MHX; M=Y→Pd; X=F,Cl.	9746	PT
	$[PdCl_4]^{2-}$. Cl exchange.	7409	DFT
	$Pd_3 + H_2$.	7363	PP
	$Pd_n + H_2$, n=2,3.	7136	PP
	PdMgO, PdOMg.	8715	PP
	M_4 on MgO(001) surface; M=Ni,Pd.	8860	DFT
	Pd, Pd_4 on MgO(001) surface.	10302	DFT
	PdCO, $PdCH_3$.	7743	PP
	$Pd(CO)_2$, $Pd(CO)_2F_2^{2-}$.	8746	PP
	$M(CO)_4$; M=Ni,Pd.	10084	PP
	CO insertion into M-H and M-CH_3 bonds, M = Y→Pd.	6969	PT
	$Pd(NO)(CH_3)(PH_3)$ + CO substitution reaction.	7744	PP
	Reductive elimination of $Pd(XH_3)(\eta^3\text{-}C_3H_5)(PH_3)$; X=C-Sn.	6959	PP
	Small hydrocarbons +M, M=Y→Pd.	7128	PT
	M + C_2H_2; M=Y→Pd.	9744	PP
	MX_2; M=Y→Pd; X=H,F,Cl.	9745	PP
	MH_2, MHX; M=Y→Pd; X=F,Cl.	9747	PP
	M-CH_3, M-C_2H_3, M-C_2H; M=Y→Pd.	9748	PT
	$MH_n + H_2$, CH_4; M=Y→Pd.	9750	PP
	$PdCl_2(H_2O)_n$, $PdHCl(H_2O)_n$.	9751	PP
	$CH_4 + M^+$; M=Y→Pd.	6971	PP
	Pd_2 + CO.	7366	PP
	Pd_2, PdCu or Cu_2 + CO or NO.	9415	PP
	Pd_2 +C_6H_6. Pd_2 +C_6H_6/Ag.	8020	PP
	$PdCl_4^{2-}$.	9839	PP
	$Pd(H)_2(Cl)(NH_3)^-$, $Pd(H)_2(NH_3)_2$.	8911	PP
	$Pd_2(\mu\text{-}Br)(\mu\text{-}C_3H_5)(PH_3)_2$, $PdCl(\eta^3\text{-}C_3H_5)(PH_3)$.	9540	PP
	M=CH_2^+; M=Y→Pd.	7627	PP
	$PdCH_2I^+$. Strong Pd-C bond.	9627,9628	DFT,PP
	$[L_2MCH_3]^+$ + ethylene reaction.	7776	PP
	Nucleophilic attack on cationic η^3-allylpalladium complexes.	7940	PP
	Pd acetate catalyzed Wacker reaction.	8464	PP
	Pd acetate catalyzed acetoxylation of ethene.	8465	PP

Element	Compounds	Ref.	Method
	Solid $(Me_4N)[M(dmit)_2]_2$; M=Ni,Pd, 'dmit' = 2-thioxo-1,3-dithion-4,5-dithiolate.	8938	PP
47 Ag	Ag_2.	9502, 10329	PP
	Ag_n, Ag_n^+.	7006–7009	PP
	Ag_3 hfs.	7050	DSW
	Ag_6.	7810, 7811	PP
	Ag_7.	6722	MS
	Ag_7.	7024	DFT,PP
	Ag_n; $n \leq 9$.	9287	PP
	M_n; M=Ru,Pd,Ag; n=55,135,140.	8183	PP
	M_4 on MgO(001) surface; M=Cu,Ag.	8860	DFT
	AgH.	8949	DF
	AlAg.	6863	PP
	AgF.	9358	PP
	AgF. RI-MP2.	10192	PP
	Solid AgX; X=Cl-I.	9076, 9077 10135	PP
	$(Ag_nBr_p)^{\pm}$; $n, p \leq 2$.	9335	PP
	AgO^+, $[AgO\{N(=CH_2)(CH_3)\}_2]^+$.	7321	
	AgHe.	8158	PP
	HeAgHe.	9220	PP
	AgCO.	8798	DK
	$AgNH_3^{0/+1}$.	9405	PP
	$M_n(NH_3)$; M=Cu,Ag; n=1-4.	7148	PP,DFT
	M-NO_2; M=Cu,Ag.	9421	PP
	$Ag(CN)_2^{q-}$; q=1,2.	9382	PP
	M_2X_2; M=Cu,Ag; X=Cl-I.	7596	PP
	$[Ag_2Br_2](PH_3)_3$.		
	Ag_2-L; L=NH_3, CO, C_2H_4, H_2O.	7030	PP
	M^+L; M=Cu,Ag; L=H_2O, OH^-, CO.	7884	PP
	Sulfur oxide anions adsorbed on Ag cluster models	9090	PP
	Ag^+-L for 18 ligands.	8753	PP
	$Ag(C_6H_6)_n^+$; n=1,2.	8754	PP
	Ag^+ + benzene, other hydrocarbons.	8031	PP
	M^+-C_5H_5N N-M complexes; M=Cu,Ag. HF/MP2/B3LYP.	10272	PP
	$(Ag^+)_n$ + butadiene complex, n=1,2.	9108	PP
	Ag_2 + olefin + O, O_2. Oxidation, epoxidation model.	9023	PP
	Ag_4 + C_6H_6.	8020	PP
	$[Ag_4(\mu_4\text{-E})]^{2+}$, its diphosphine complex. E=S-Te.	10157	PP
	Ag_4Ph_4	6897	DFT
	$[Ag(NHCHNH)]_2$, $[Ag(dmtp)(NO_3)]_2$.	7597	PP
	Bimetallic cluster $[Ag_{13}\{Fe(CO)_4\}_8]^{n-}$, n=0-5.	6627	DFT
	M-$(Mg_{13}O_{12})$ surface model; M=Rb,Pd,Ag.	7690	PP
	M_n-MgO(001); n=2,4; M=Pd,Ag.	7692	DFT
	Ag_2/'AgBr'.	9715	PP
	HCHO + Ag_2.	9718	PP
	MgO(100)/Ag(100) and MgO(110)/Ag(110) interfaces.	9300	PP
	Solid DCNQI-M; M=Cu,Ag; DCNQI=dicyanoquinonediimine.	8939	PP

Element	Compounds	Ref.	Method
	Pd_2 +C_6H_6. Pd_2 +C_6H_6/Ag.	8020	PP
48 Cd	Cd_2.	7337	PP
	CdH^q; q=-1,0,+1.	7600	DFB+CCSD
	CdRg, Rg=He-Xe.	7342	PP
	MO, MO_2; M=Zn,Cd.	7208	PP
	CdE; E=S-Te. Nanocrystalline clusters. SO.	9988, 9990	PP
	MX_2, $(MX_2)_2$; X=H,F-I.	8309	PP
	CdX_2; X=F,Cl. $CdF_2Cl_2^{2-}$. EFG. CCSD(T).	8002	PT
	Cd-(en), Cd-NH_3 exciplexes. 'En'=ethylenediamine.	9925	PP
	Cd + CH_4.	9359	PP
	Cd + H_2.	9360	PP
	Cd^+ + C_6H_6.	8031	PP
	M^{2+}L; M=Zn,Cd; L=H_2O, OH^-, CO.	7884	PP
	M^{2+}:M'O; M=Cu,Ag; M'=Mg-Sr. Impurities.	9171	PP
49 In	InR, $(InR)_4$; R=H,Me.	10042	PP
	MeM; M=Ga,In.	8024	DFT+PP
	In_2P_2.	7676	PP
	In_3P_2, In_2P_3.	7679	PP
	In_2P, InP_2.	7680	PP
	In_3Sb_2, In_2Sb_3, their cations.	7682	PP
	$In_2As_2^n$, n = -1, 0, +1.	7683	PP
	InH, InF, InCl.	8600	PP
	InCl, $InCl_3$.	6859	DK, PP
		9639	PP
	InX_n, X=H,Cl,-CH_3; n=1-3. SR.	6860	DK
	MX_4^-; M=Ga-In; X=Cl-I. Ga, In NMR shifts.	9926	PT
	$InMH_6$, MBH_6; M=B-In.	6907	PP
	X_3M–D; M=Al-In; X=F-I; D=YH_3,YX_3,X^-; Y=N-As. Donor-acceptor complexes.	9972	PP
	Univalent ligands MeM, (Cp)M, (Cp*)M, $(H_3Si)_2NM$; M=B-In. Their $Fe(CO)_4$ complexes.	8755	DFT+PP
	In^+ complexes with H_2O, CH_3OH, other organics	6731	PP
	Hydration of Group 2 - Group 13 ions. $M(H_2O)_6^{n+}$. M=Ca→Ga, Sr→In.	6616, 6617	PP,PT
50 Sn	Solid C - Sn. Cohesive energy.	9175	PP
	SnH.	6639	PP
	MH; M=C-Sn, Te. Test SO PP program.	9924	PP
	SnF^+.	6793	PP
	SnF.	7352	PP
	Sn_5.	7359	PP
	M_5^+, M=Ge,Sn.	7361	PP
	MH_2; M=C-Sn. SO splitting.	8434	PP
	SnH_4.	7599	DF+CCSD
	SnH_4. Freq. dep. polarizability.	10129	RRPA
	MH_3 + MH_4; M=Si-Sn.	7369	PP
	MH_4; M=C-Sn. Infrared intensities.	7437	PP
	M_2, CuM, Cu_2M, CuM_2; M=Si-Sn.	9263	PP
	MX_2; M=Si-Sn; X=F,Cl.	9741	DFT
	ML_2; M=Ge,Sn; L=H, $P(SiH_3)_2$.	7508	PP

Element		Compounds	Ref.	Method
		MOH^+, HMO^+; M=C-Sn.	9422	PP
		$Sn[E(SiH_3)_2]_2$; E=N, P.	7508	PP
		HZnMH; M=C,Sn.	9556	PP
		Isomers of vinyl stannane.	8818	PP
		$(CO)_5Cr{=}MH_2$; M=C-Sn.	8153	DFT
		Reductive elimination of $Pd(XH_3)(\eta^3\text{-}C_3H_5)(PH_3)$; X=C-Sn. Hypervalent behaviour of X.	6959	PP
		M_8C_{12}; M=Si-Sn.	6988	PP
		σ-bond activation of $(HO)_2B\text{-}XH_3$ by $M(PH_3)_2$; X=C-Sn; M=Pd,Pt.	9533	PP
51	Sb	SbO.	6637	PP
		SbH.	6644	PP
		SbI.	7387	PP
		Sb_2.	7390	PP
		Ozone-like, Sb_3^{3-} compounds. M_3Sb_3; M=Na-Rb. $Na_4Sb_3^+$.	7938	PP
		Sb_4 and isoelectronic species.	7939	PP
		In_3Sb_2, In_2Sb_3, their cations.	7682	PP
		Solid EM semiconductors; E=B-In; M=N-Sb. Cohesive energy.	9176	PP
		Sb speciation in sulfidic solutions.	10000	PP
		SbF.	7031,8572	PP
		SbF_2, SbF_2^+.	8573	PP
		SbX_2, SbX_2^+; X=Cl,Br.	6792	PP
		$(Sb_nO_m)^q$, q=0,1.	8239	PP
		CH_3EH_2, $CH_2EH_2^+$; E=N-Sb.	8265	PP
52	Te	H_2Te.	8455	PP
		H_2X; X=O-Te. H and X NMR shifts. 2nd and 3rd order SO effects. SOO.	10059	PT
		H_2X; X=O-Te. NMR spin-spin coupling. 2nd and 3rd order SO effects. SOO.	10060	PT
		Tetra-atomic $(X_2)(Y_2)$ and (XY)(XY) clusters; X,Y=O-Te.	9107	PP
		MF_6, MF_6^{2-}; M=Se,Te.	8399	PP
		MCl_6, MCl_6^{2-}; M=Se,Te.	8400	PP
		$W(PH_3)_4E_2$; E=O,S,Te. W(IV), d^2.	8248	DV DFT
		$TeCl_4$.	8448,8449	PP
		CH_2EH^+; E=S-Te.	8265	PP
		$CH_2(EH)_2$; E=O-Te.	9547	PP
		CdE; E=S-Te. Nanocrystalline clusters. SO.	9988,9990	PP
		$Te(SR)_2$; R=H,Me. $Te(SH)_4$ thermodynamically unstable.	7716	PP
		$HX\text{-}CH_2\text{-}CHO$; X=S-Te. No significant X...O interactions.	8813	PP
		$[C(ER)_3]^+$; E=O-Te.	9084	PP
		X_2Y_2; X=N-Sb; Y=O-Te. Planar or butterfly?	8889	PP
		$CH_3 + CH_3EH$; E=S-Te.	9776	PP
		$C_6H_4S_2Te$.	9622	PP
		$HESi(SiH_3)_3$; E=O-Te. Photoelectron spectrum.	9970	PP
		Vibr. freq. of TM chalcogenides; M=Ti...Os; Ch=O-Te.	7325	PP
		^{125}Te NMR shifts.	9483	SR DFT
53	I	I_2, I_2^-, I_3^-, I_5^-.	7374,9713	PP
		I_2 excited states.	9952	PP
		I_2. HF to CCSD(T) level.	7418	DF

Element	Compounds	Ref.	Method
	I_n^-; n=3,5.	9897	PP
	X_2; X=F-I. 7-VE PP.	7472	PP
	X_2, HX; X=F-I	7473	PP
	I_2, HI. Spin-orbit effects via ZORA.	10077	DFT
	Interhalogens up to IBr. Up to CCSD.	7416	DF
	Interhalogens up to IBr. Up to CCSD(T).	9186	PT
	HX, XY, X_2 complexes with NH_3. X,Y=F-I	10338	PP
	IF	7106	PP
	IF and ICl. SR transition moments for B $0^+(^3\Pi) \rightarrow$ X 0^+ ($^1\Sigma^+$).	10303	PP
	I_2^-, ICl^-. Ground and excited states.	8846	PT
	X_3^+, XY_2^+; X,Y=F-I	8621	PP
	Ar·I_2 ground-state potential. Linear and T.	8496	DK
	I·CO_2, I·OCS van der Waals complexes.	9557	PP
	Solid MX; M=Li ... Rb; X=F ... I.	7486	PP
	$Na_nX_m^q$; X=Cl-I; q=0,+1. n=1-3, m=1-2.	10203	PP
	CaI^{2+}.	6645	PP
	CuX^-; X=F-I. Cu_5-I^-.	8097	PP
	GaX_2, GaX_3, X=Cl-I.	7349	PP
	HX, CH_nX_{4-n}; X=F-I. SO-induced ^{1}H, ^{13}C NMR shifts.	8774	DFT
	HX, CH_3X; X=F-I. SO-induced ^{1}H, ^{13}C NMR shifts. Importance of two-electron SO terms.	8775	DFT
	HX, CH_3X. ^{13}C NMR shifts. SO.	10221	DFT
	HX; X=Cl-I. EFG.	8326	PT,DK
	HX; X=Cl-At. Picture-change effect on EFG.	8327	
	HX, CH_3X; X=F-I. ^{1}H and ^{13}C NMR shifts.	9026	PT
	HX, CH_3X; X=F-I. H, C and X NMR shifts. 2nd and 3rd order SO effects.	10059,10061	PT
	HX; X=F-I. NMR spin-spin coupling. 2nd and 3rd order SO effects. SOO.	10060	PT
	HX; X=F-I. NMR shielding and spin-spin coupling.	10124	RRPA
	EFG in HX; X=Cl-I. MP2 to CCSD(T). R/NR.	10125	DF+corr.
	HI, CH_3I.	8371	PP
	HI. Frozen-core DF test.	10182	DF
	Pseudopot. vs. all-electron on Br, I compounds. G2 set.	7839	PP
	CH_3I SO splitting.	9920	PP
	CX_3^+; X=F-I. ^{13}C NMR shifts.	8298	DFT+PP
	CX_4, CX_4^-; X=Cl-I. PES.	9458,9461	PP
	CF_3I Rydberg levels. SO.	9918	DFT
	CD_3X; X=F-I. Deuterium EFG.	10058	PP
	EtX; X=F-I.	8098	PP
	IF^+, ICF_n^+; n=1-3.	7674	DFT+PP
	CF_3X^-; X=Cl-I.	9459	PP
	AlX_4^-; X=H,F-I. ^{27}Al NMR shifts.	9022	PT
	PX_4^+; X=F-I ^{31}P NMR shifts. SO.	8292	DFT+PP
	CF_3IF_n; n=0,2,4,6. ^{13}C and ^{19}F NMR shifts.	8300	DFT+PP
	Iodo-organic compounds. ^{1}H and ^{13}C NMR shifts. SO analyzed.	8301	DFT
	I_2HSi-SiH_2I.	8193	PP

Element	Compounds	Ref.	Method
	$I(N_3)_2^+$.	9996	PP
	X-N_3; X=H,F-I.	9624	PP
	ICN, INC.	9549	PP
	HOX; X=F-I.	7840	PP
	XO_n^-; X=Cl-I; n=1-4.	9080	PP
	H_2CI_2 isomers.	7838	PP
	PI_2, PI_2^+.	8575	PP
	$P_2I_5^+$.	6746	PP
	BX_2, BX_2^+, X=Br,I.	8593	PP
	$I(N_3)$.	7098	PP
	$PdCH_2I^+$.	9628	PP
	IF_4^-, IF_5^{2-}.	7231	PP
	AlX_4^-; X=F-I. Al NMR shift.	9022	PP
	SiX_4, $SiXI_3$. Si NMR shift.	9025	PP
	TiX_4; X=Br-I. PES.	9020	PP
	TiX_4; X=F-I. Ti NMR shift.	9024	PP
	NbX_6^-, $NbCl_5X^-$; X=F-I. Nb NMR shift.	9024	PP at X
	IOF_5.	7226	PP
	IOF_6^-, IF_7, XeF_5^-.	7228	PP
	TeF_7^-, IF_7, XeF_7^+ are D_{5h}.	7230	PP
	$XONO_2$; X=F-I.	7570	PP
	CH_2X^+; X=F-I.	8265	PP
	S_N2 reaction X^- + CH_3X, X=F-I.	7434	DFT
	$I^- \cdot CH_3I$.	8066	PP
	Reactions of iodo-lithio-ethenes.	7116,7117	PP
	$C_6H_4X^-$ (benzyne + halide); X=F-I.	8973	PP
	$C_6H_6 \cdot I_2$ complex.	8877	PP
	Vibr. freq. of 50 inorg. molecules as test of PP.	7102	PP
	$I(^2P_{3/2})+O_2(a\ ^1\Delta_g) \leftrightarrow I(^2P_{1/2})+O_2(X\ ^3\Sigma_g^-)$.	8244	PT
	Hydrated halogenide complexes. AE/PP.	8519	PP
54 Xe	RgH^+; Rg=Ar-Xe.	8735	PP
	RgH; Rg=Ne-Xe.	8359	PP
	XeH. Low-lying states.	10023	PP
	XeX^q; X=F-I; q=-1,0,+1.	9617	PP
	XeO, XeS. Low-lying states.	10256	PP
	$RbXe^+$.	6791	PP
	BRg^+; Rg=Ar-Kr.	8436	PP
	$(Rg)_2$; Rg=Ne-Xe	7088,9437	PP
	$(Rg)_2$; Rg=Kr,Xe	8940	PP
	CdRg, Rg=He-Xe.	7342	PP
	$RgNO^+$; Rg=He-Xe	8592	PP
	$RgAu^+$, $RgAuRg^+$; Rg=He-X. First Au-Rg bonds predicted.	9303	PP
	RgBeO; Rg=Ar-Xe	10096	PP
	HXeH	9231,9488	PP
	RgF_2; Rg=Kr,Xe	7093	PP
	XeF_2.	8800	PP
	XeF_4	7094	PP
	XeF_n; n=2,4,6.	9848	DFB

Element	Compounds	Ref.	Method
	$[XeOF_5]^-$	7229	PP
	$XeHXe^+$	9058	PP
	$RgHRg^+$; Rg=Ar-Xe.	8738	PP
	$Xe_2H_3^+$ ($HXe{\cdot\cdot}H{\cdot\cdot}XeH^+$).	8734,8737	DFT+PP
	HXeCl.	8196,9232	PP
	HXeOH.	9227	PP
	HXeSH.	9229	PP
	HKrCN, HXeCN, HXeNC.	9228	PP
	FXeX; X=N_3,NCO,OCN.	9623	PP
	F_2C=C-Xe.	9552	PP
	HXeX; X=Cl-I. HKrCl.	9230	PP
	$RgHX^+$; Rg=Ar-Xe; X=Cl-I.	8739	PP
	$C_6F_5Rg^+$; Rg=He-Xe.	7786	PP
	XeF^+, $XeCF^+$, $XeCF_2^+$. Cleavage of C-F bonds.	7674	DFT+PP
	XeH_2 - H_2O dihydrogen-bonded (O-H··H-Xe) complex.	8736	PP
	$M(CO)_5$-Rg; M=Cr-W; Rg=Ar-Xe.	7576	PP, DFT
55 Cs	MH; M=Li-Cs.	7471	PP
	MF, M=K-Cs.	7533,8599	DF/PT/HF;PP
	CsF. Q(Cs) obtained.	9190	DK CCSD(T)
	CsAu.	9573	DF/HF
	ML; M=Li-Cs; L=H,Me,NH_2,OH,F,Cp.	8561	PP
	M_nX_m; M=Li-Cs; X=Se,Te, $n,m \leq 2$.	8095	PP
	M_nX_m; M=Li-Cs; X=As,Sb, $n \leq 2$, $m \leq 4$.	8096	PP
	CsRg; Rg=Ne-Xe.	7569	PP
	M^+-CO; M=Li-Cs.	7691	PP
	M^+-L; M=Li-Cs; L=adenine, guanine.	7087	PP
56 Ba	Ba_2.	6657	PP
	Ba_n, n=2-14.	7033	PP
	Solid Ba.	10318	PP
	BaLi.	6656	PP
	BaRg; Rg=He-Xe.	7336,7338	PP
		7341	
	BaH^+.	6658	PP
	BaI^{2+}.	6646	PP
	MX_2; X=H,F; M=Ca-Ba.	7101	PP
	MX_2; M=Sr,Ba; X=F-I. All floppy; SrF_2 and BaF_2 to $BaBr_2$ are bent.	8937	PP
	MCN, MNC; M=Be-Ba.	8570	PP
	$M(CN)_2$, M=Be-Ba.	8266	PP
	MH, M_2H_4; M=Mg-Ba.	8304	PP
	M^{2+}-L; M=Mg-Ba; L=adenine, guanine.	7087	PP
	$MCl_2 \cdot nH_2O$; M=Sr,Ba; n=1,2. Madelung potential.	8961	PP
	Hydrated M^{2+} + adenine, thymine base pairs; M=Mg-Ba.	9809,9810	PP
	$Ba_6Li_3O_2$ cluster with ligands.	6986	DFT
57 La	La_n; n=2-13. Used to derive potential for MD simulations.	7628	DFT-DVM
	LaO, LaO^+.	8819,9585	PP
	MO^q, MO_2^q, MO_3^q species; M=Y,La.	6680	DFT,PP
	LaX_3, X=F,Cl.	7454	PP
	LaX_3; X=Cl-I.	8451	PP

Element		Compounds	Ref.	Method
		MF_6^{3-}; M=Sc,Y,La.	7922	PP
		Cp_2LaL; L=$CH(SiH_3)_2$.	7453	DFT,PP
		LaC_2.	9453	PP
		LaC_n^+; n=12,13.	9454	PP
		LaC_n; n=2-6.	9455	PP
		LaC_n; n=2-8.	10234	PP
		LaC_2, LaC_2^+.	10236	PP
		LaC_3^{q+}; q=1-3.	10235	PP
		MC_n; n=3-6; M=Y,La.	9846	PP
		$La@C_{82}$.	9266	PP
58	Ce	CeO.	7450,9531	PP
		CeO, CeF.	7346	DFT
		CeO^+, $CeO_2^{0/+1}$.	7986	PP
		MO_8^{12-}; M=Zr,Ce. Models for solid MO_2.	9017	DV DFT
		Ce^{n+} in alkaline-earth fluorides.	10133	DF
		CeX_n, n=3,4; X=F,Cl.	8569	PP
		$NaCeCl_4$.	8261	PP
		$Ce(Cp)_3$, $4f^1$.	8255	DV DFT
		$Ce@C_{28}$. f-Orbital covalency.	9435	DFT
62	Sm	Sm(III)-catalyzed olefin hydroboration.	8490	PP
		Ethylene insertion into Sm-C bond of $H_2SiCp_2SmCH_3$.	8413	PP
		SmF_6^{4-} cluster models.	7510	
63	Eu	Diatomic EuE; E=O-Te. $5d$ important.	7345	DFT
		$[EuO_6]^{9-}$ +Madelung cluster model for Eu^{3+} in Ba_2GdNbO_6. The f^6 spectrum.	7460	DF
64	Gd	GdF. DF. Gd $5d \rightarrow$F $2p$ donation, F $2s$ - Gd $5p$ hybridization.	9948	DF
		GdF_2.	9949	DF
		$[Gd(H_2O)_9]^{3+}$.	7281	PP
		$M(C_6H_6)_2$; M=Y,Gd.	7455	PP
		Gd(III) polyamino carboxylates.	7282	PP
67	Ho	Ho_2.	9048	PP
		C-F bond activation by Ln^+; Ln=Ce,Ho.	8011	PP
69	Tm	LnF_n; Ln=Er,Tm; n=1-3.	8603	PP
70	Yb	Yb_2.	10172	PP
		Yb_n; n=3-7.	10173	PP
		LnO; Ln=La ... Yb. YbF. R/NR.	10164	DFT
		LnO, LnF; Ln=Ce ... Yb.	7483	PP
		LnO, LnS; Ln=Eu,Yb.	8691	DFT
		YbF. PNC experiment.	8982,9974	PP
		YbF. PNC.	9162,9332	DF
		YbH,YbF,YbO.	8689	PP
		L$\rightarrow Ln^{3+}$, Ln=La,Eu,Yb; L = [R_3P=O], amides, pyridine.	6921	PP
		Dithiophosphinate Ln^{3+} complexes. Ln=La ...Yb.	6992	PP
		$Ln(C_8H_8)_2$; Ln=Nd,Tb,Yb. Excited states. Lanthanocenes are $4f^n\pi^3$, actinocenes $5f^{n-1}\pi^4$.	8687	PP
		$Ln(C_8H_8)_2^-$; Ln=Ce,Nd,Tb,Yb. Excited states.	8688	PP
71	Lu	LnH, LnF, LnO; Ln=La,Gd,Yb,Lu. Lanthanide contraction.	10165	DFT
		LnH, LnF, LnO; Ln=La,Lu. Lanthanide contraction.	8485	PP

Element	Compounds	Ref.	Method
	LnO, $LnO^{\pm}$, LnO_2, LnO_2^-, LnO_3^-, $(LnO)_2$. Ln=Ce-Lu.	10218	DFT
	MF, MH, MH_3; M=La,Lu,Ac,Lr. Lanthanide and actinide contractions.	8550	DF+MP2
	LnX_3; Ln=La-Gd,Lu; X=F,Cl.	8568	PP
	LnX_3; Ln=La,Gd,Lu; X=F-I. DFT vs. MCSCF or CISD+Q.	6590,6591	PP,DFT
	LnX_3; Ln=La-Lu; X=F,Cl.	8229,8230 10021	PP
	LnX_3; Ln=Ce-Lu; X=F-I.	7327	PP
	$Ln(C_6H_6)_2$, Ln=La ... Lu.	8047	PP
	$Ln(C_6H_6)_2$, Ln=La ... Lu. R/NR. Dominated by Ln $5d \rightarrow \pi^*$ back donation.	8721	DFT
	Ln-CO, Ln-OC; Ln=La,Gd,Lu.	8046	DFT
	$M_2@C_{80}$; M=Sc,Y,La,...Lu.	8406,8408	PP
	$M@C_{82}$; M=Sc,Y,La,...Lu.	8407	PP
72 Hf	R/NR orbital energies for M_6, M=Ti-Hf.	6589	DFT
	Hf_3.	7367	PP
	MH_n; M=Zr,Hf; n=1-4.	7206	PP
	MCl_4; M=Ti-Hf. Vibr. freq.	9489	PP
	MF_4; M=Ti-Hf. PES.	7535	DFT
	$HfCl_4$. PES.	8251	DFT
	MX_4; M=Ti-Hf; X=Cl,Br.	8694	DFT
	MX_4; M=Zr,Hf; X=Br,I. PES.	9871	SR SW
	HfX_6^{2-}; X=F-I. Salts	7923	PP
	MN, NMN, $M(N_2)$, $M(\mu\text{-}N)_2M$; M=Ti-Hf.	8507	PP
	MMe_2Cl_2; M=Ti-Hf. Bent's rule for bond angles	8208	PP
	$[MMe_6]^{2-}$; M=Ti-Hf. Non-octahedral	8289	PP
	$Cp_2M=E$; M=Ti-Hf; E=O-Te.	6911	PP
	$H_2(X)M\text{-}NH_2 \rightarrow H_2M{=}NH + HX$; M=Ti-Hf; X=H,Cl, Me,$NH_2$,$SiH_3$.	7320	PP
	$H_3M\text{-}EH_3$, $H_2M{=}EH_2$; M=Ti-Hf; E=C-Sn.	7324	PP
	$[MCp(CO)_4]^-$; M=Ti-Hf. ^{13}C NMR shifts.	8283	PP
	$M(C_6H_6)_2$; M=Ti-Hf.	8375	PP
	$Hf@C_{28}$.	10024,10025	PP
	$Hf@C_{28}H_4$.	10026	PP
73 Ta	MO; V-Ta.	9349	PP
	TaL_5; L=H,Cl,Me. Which structure?	8260	PP
	TaF_6^-.	7922	PP
	Heptoxides $M_2O_7^{4-}$, M=V-Ta.	6667	PP
	Ta + CO.	8764,9938	PP
	CMO^-, OMCCO, $(C_2)MO_2$, $M(CO)_n$; n=1-6; M=Nb,Ta.	10348	DFT+PP
	$Ta^+ + CH_4$.	9553	PP
	TaC, TaC^+.	8770	PP
	TaC_2^+.	8768,9457	PP
	TaC_n^+; n=7-13.	9456	PP
	MN_n; M=Nb,Ta; n=1-3.	10345	DFT+PP
	$[MMe_6]^-$; M=V-Ta. Non-octahedral	8289	PP
	$[Ta(OH)_2L'(H_2)L]^+$; L=PH_3; L'=F^-,Br^-,I^-,CO,CN^-, ...	6871	PP
	$M(NH_2)(=NH)_2$; M=V-Ta imido adducts of CH_4.	7312,7314	PP

Element	Compounds	Ref.	Method
	$Cl_3Ta{=}E$; E=MH_2 (M=C-Sn), MH (M=N-Sb), M (M=O-Te).	6910, 6911	PP
	$[Cp_2TaH_3]$.	7111	PP
	$[MCp(CO)_4]$; M=V-Ta ^{13}C NMR shifts.	8283	PP
74 W	W_3.	6790	PP
	Octahedral M_6, M=Mo,W.	6714	MS
	$W_6X_8X_6^{2-}$; X=Cl-I.	6717	MS
	WF_4. Lowest triplet state.	7921	PP+DFT
	WL_6; L=H,F,Me. Which structure?	8260	PP
	WX_6; X=H,F.	9944	PP
	MF_6; M=Mo,W.	9169	SR SW
	WH_6. C_{3v}, not O_h!	9719	PT
	WH_6.	8013	PP
	WMe_6. Distorted, C_3 structure.	8286	PP
	$[MMe_6]$; M=Cr-W. Non-octahedral	8289	PP
	WMe_nCl_{6-n}; n=1-3.	8290	DFT+PP
	WF_4 triplet state	7921	PP
	$[MS_6]^{8-}$ cluster models for MS_2 solids; M=Ta,W	7384	MS
	MO_2Cl_2; M=Cr-W. Vibr. freq.	9489	PP
	$[M_2Cl_9]^{3-}$; M=Mo,W.	9841	DFT
	$WO_nS_{4-n}^{2-}$; n=0-4, WX_6; X=F,Cl,CO. ^{183}W NMR shifts.	9420	DFT
	MS_4^{2-}; M=Mo,W. Excited states.	9872	SR SW
	$MS_4^{2-/3-}$; M=Mo,W. Redox energy in vacuum.	10306	DFT,PP
	$M_3X_4^{4+}$; M=Mo,W; X=O,S.	8622, 8623	PP
	$M_2O_7^{2-}$; M=Cr-W.	6667, 8895	PP
	MO_2^-; M=Cr-W.	10346	DFT+PP
	Solid WO_3.	7271	PP
	M + CO; M=Mo,W.	9937	PP
	$M(CO)_6$; M=Cr-W.	7378, 7573, 7574	PP
	$M(CO)_6$; M=Mo,W.	9037	SR DFT
	$M(CO)_6$; M=Cr-W.	8616, 8617	DFT
		9613	
	$M(CO)_6$; M=Cr-W. Electronic spectra.	9432	DFT
	$M(CO)_6$; M=Cr-W	8209	PP
	MO_4^{2-}, $M(CO)_6$; M=Cr-W. O NMR shifts.	9611	SR DFT
	$M(CO)_6$; M=Cr-W. C and O NMR shifts.	8296	DFT+PP
	$M(CO)_6$; M=Cr-W. C and O NMR shifts. SR/NR.	9482	DFT
	$M(CO)_6$; M=Cr-W. HOMO electron density.	9424	PP
	$W(CO)_6$ as test of ZORA geometry optimization.	10076	DFT
	$M(CO)_6$; M=Cr-W.	10088	DFT
	$(CO)_5M{=}CH_2$; M=Mn^+,Mo,W.	8153	DFT
	$M(CO)_5$-Rg; M=Cr-W; Rg=Ar-Xe.	7576	PP, DFT
	$W(CO)_n^+$; n=1-6.	7080	PP
	WCl_4L, WCl_5L^-, $W(CO)_5L$; L=acetylene, ethene.	9239	PP
	$[Cl_3M{\equiv}N]_n$; M=Mo,W; n=1-6 rings.	9604	PP
	$M(CO)_5CX$; M=Cr-W; X=O-Se.	6915	DFT
	$M(CO)_5L$; M=Cr-W; L=CO, SiO, CS, N_2, NO^+, CN^-, NC^-, HCCH,CCH_2, CH_2, CF_2, H_2.	7572	PP
	$[(HO)_3W{\equiv}P]$, $[(HO)_3W{\equiv}P{\rightarrow}W(CO)_5]$, $[(thf)(HO)_3W{\equiv}P{\rightarrow}W(CO)_5]$.	8468	PP

Element	Compounds	Ref.	Method
	$W(CO)_5NH_3$.	10309	PP
	MN, NMO, $MNO^{\pm}$; M=Mo,W.	6679	PP
	MO_2^{2+}, MN_2, MP_2; M=Mo,W.	9315	PP
	Supported nitrido dimers and trimers of W.	7214	PP
	$WC_2H_2^+$.	7819	PP
	Mixed-ring sandwich $[M(\eta^7\text{-}C_7H_7)(\eta^5\text{-}C_5H_5)]$; M=Ti,V-Ta. Cp bonding more ionic, cycloheptatrienyl more covalent.	8249	DFT
	Cp_2M, Cp_2MO, $Cp_2MCl(OSiH_3)$; M=Mo,W.	8743	PP
	$[MCpMe(CO)_3]$; M=Cr-W ^{13}C NMR shifts.	8283	PP
	Metallacyclophosphazenes $MCl_3[N_3(PH_2)_2]$; M=Cr-W. Metallacyclothiazenes $MCl_2[N_3S_2]$.	9881	DFT+PP
	$[M(CO)_5L]$; M=Cr-W; L=PH_3, PX_3 ^{31}P NMR shifts	8285	PP
	$[M(CO)_5L]$; M=Cr-W; L=OH_2,NH_3,PH_3,PMe_3,N_2,CO;OC,CS, CH_2,CF_2,CCl_2,NO^+. Discusses 'trans effect'.	10087	DFT
	$[Cp(CO)_2M]_2(\mu\text{-}E)$; M=Cr,W; E=S-Te.	8179	PP
	$[WL_2(\mu\text{-}CR)]_2$; L=H,Me,F,OH; R=H,F,Me.	8177	PP
	$(CO)_5M{=}CH_2$; M=Cr-W Fischer carbenes.	8151	DFT
	Low-valent (Fischer) carbenes $[(CO)_5W{=}CH_2]$, ... high-valent (Schrock) carbenes $[X_4W{=}CH_2]$,...; X=F-I.	10148	PP
	Low-valent (Fischer) carbynes $[F(CO)_4W{\equiv}CH]$, ... high-valent (Schrock) carbenes $[X_3W{\equiv}CH]$,...; X=F-I.	10149	PP
	$M(PMe_3)_4X_2 + H_2$; M=Mo,W; X=F-I.	7968	DFT+PP
	$M(=NH)_3$; M=Mo,W imido adducts of CH_4.	7312	PP
	$W(OH)_2(=NH) + CH_4$.	7313	PP
	$Cl_4W{=}E$; E=MH_2 (M=C-Sn), MH (M=N-Sb), M (M=O-Te).	6910,6911	PP
	d^1 systems MEX_4^{z-}; M=V,Cr-W,Tc-Re; E=O,N; X=F-Br. g-tensors.	9173	DFT
	$[(N_3,N)WL]$, L=Cl, P-BH_3, $\equiv$E; E=N-Sb. $(N_3,N) = N(CH_2CH_2NSiMe_3)_3$.	9588	PP
	MO_2X_2; M=Cr-W; X=F-Br.	6911	PP
	$W(CO)_3(PH_3)_2(H_2)$. Classical or non-classical?	9985	PP
	$M(CO)_n(PH_3)_{5-n} + H_2$; M=Cr-W; n=0,3,5.	9986	PP
	W-Al bonds and other TM–main-group bonds.	7750	PP
	Phosphinidenes $M(CO)_5$-PR; M=Cr-W; R=H,Ph,OH,NH_2.	7577	DFT
	$[Cp_2MH_3]^+$; M=Mo,W.	7111	PP
	$X_4M(HCCH)$; M=Mo,W; X=F,Cl vinylidene rearrangement.	9826,9827	PP
	$M(C_6H_6)_2$; M=Cr-W.	8375	PP
	$[W(OH)_2(C_6H_6)(Ph_3)] + N_2H_2$ 4e reduction.	8845	PP
	$W(PH_3)_4E_2$; E=O,S,Te. W(IV), d^2.	8248	DV DFT
	Trans-$M(PH_3)_4E_2$; M=Mo,W; E=O,S,Te. W(IV), d^2.	8366	DFT
	$M_6S_8L_6$ clusters, M=Mo,W.	6713	MS
	$W_2(OR)_6$ + alkynes;R=H. Relativistic effects crucial.	7657	DFT
75 Re	$HM(CO)_5$, M=Mn,Re.	8210	PP
	ReH.	7348	PP
	ReN, ReN_2.	10345	PP
	Heptoxides M_2O_7, M=Mn-Re.	6667	PP
	MS_4^{n-}; M=Mo,W,Re. ESCA spectra.	8991	SR SW
	$MS_4^{1-/2-}$; M=Tc-Re. ReS_4^{3-}. Redox energy in vacuum.	10306	DFT,PP
	$ReNi_{12}H_2 + H_2$. Re-doped heterogeneous catalyst model.	9899	DFT

Element	Compounds	Ref.	Method
	$Re_6S_8X_6^{4-}$; X=Cl-I.	6719	MS
	$Re_6Se_8X_6^{4-}$; X=Cl,I.	6721	MS
	d^1 systems MEX_4^{z-}; M=V,Cr-W,Tc-Re; E=O,N; X=F-Br. g-tensors.	9173	DFT
	d^2 complexes with $[M(NAr)_2]$ cores; M=W,Re. Isolobality of MCp_2 and $M(NR)_2$.	10215	SW DFT
	M + CO; M=Tc-Re, Ta.	9938	PP
	Addition of $LReO_3$, L=O^-,Cl,Cp, to C_2H_4.	7445	
	Epoxidation of ethene by $MeRe(O)_2(O_2)$, $MeRe(O)(O_2)_2$ +water.	10233	PP
	MO_3, MO_3^+, $CpMO_3$, $M(CO)_3$; M=Mn-Re.	9917	PP
	MO_3X; M=Mn-Re; X=F-Br,Me.	6911	PP
	RMO_3; R=Me,Ph,Cp; M=Tc,Re. PES.	8437-8439	DFT
	$LReO_3$; L=Me,Ph,Cl,F,OH,NH_2. Oxygen transfer to PPh_3. $(CH_3ReO)_2(\mu\text{-}O)_2$.	7827,7829	DFT+PP
	$CpReO_3$, MCl_4E; M=Cr-W,Re; E=O-Te: Metal-chalcogen multiple bonds.	7851	DFT+PT
	Metallacyclophosphazenes $MCl_3[N_3(PH_2)_2]$; M=Tc-Re.	9881	DFT+PP
	$[Cp(CO)_2M]_2(\mu\text{-}E)$; M=Mn,Re; E=S-Te	8179	PP
	$L_4Re\overset{4}{=\!=}ReL_4$	6962,6965	PP
	$HRe(CO)_3(DAB)$; DAB=1,4-diaza-1,3-butadiene. Optical spectrum. MCSCF required for the quadruple bond.	7912	PP
	Allylic rearrangement of allyloxo metal oxo complexes. M=Ta,Re.	6899	PP
	Re(O) acetylides, $ReOCl_4^-$, $ReOF_5$.	7317	PP
	$[(C_6H_6)M(CO)_3]^+$: M=Mn-Re.	7262	PP
	$[MMe_6]^+$; M=Tc,Re. Non-octahedral.	8289	PP
	Lewis basicity of $Cl_2(PH_3)_3ReN$-L complexes.	10150	PP
	$M(H)(CO)_3$(H-DAB); M=Mn,Re; H-DAB = 1,4-Diaza-1,3-butadiene. SO effects on the M-H bond homolysis.	7370	PP
	MH_n^q, MMe_n^q; M=Zr,TcTa,W,Re. Molecular shapes.	8566	PP
76 Os	R/NR orbital energies for M_6, M=Fe-Os.	6589	DFT
	OsN.	9353	PP
	OsO_4. 5p SO influence on valence PES.	9306	PP
	OsO_4. Vibrations.	9489,9997	PP
	OsO_4. RI-MP2	10192	PP
	MO_4, M=Ru, Os. PES.	6712	MS
	MO_4, M=Ru, Os. PES.	7876	PP
	OsO_4, OsO_3F_2, ..., OsF_8.	10094	PP
	OsO_4. SO effects on PES.	7096	DFT
	MO_4; M=Ru-Os. O NMR shifts.	9611	SR DFT
	$MS_4^{0/1-}$; M=Ru-Os. OsS_4^{2-}. Redox energy in vacuum.	10306	DFT,PP
	^{17}O NMR shifts in MO_4; M=Fe-Os, MnO_4^-; M=Mn-Re,	8299	DFT+PP
	MO_4^{q-}; M=V...Os. Excited states. MO_4^{2-}; M=Cr-W.	9847	DFT
	Nonlinear optical properties of MO_4^q; M=Ti...Os.	7323	PP
	Vibr. freq. of TM chalcogenides; M=Ti...Os; Ch=O-Te.	7325	PP
	$OsO_4(NR_3)$.	10043	PP
	OsCO.	9936	PP

Element	Compounds	Ref.	Method
	MCO^+, $M(CO)_n^q$; M=Ru,Os; n=1-4; q=-1,0.	10347	DFT+PP
	$Os(CO)_4H_2$, metallacyclophanes.	10179	PP
	$M(CO)_5$; M=Fe-Os.	7575	PP
	$M(CO)_5$; M=Fe-Os.	8209	PP
	$M(CO)_5$; M=Fe-Os.	9613	DFT
	$M(CO)_5$; M=Fe-Os. DFT by DPT.	10085	DFT
	$M(CO)_5$, $M(CO)_4(C_2H_2)$; M=Fe-Os.	7405	PP
	$Os(CO)_5$ as test of ZORA geometry optimization.	10076	DFT
	$[M_nC(CO)_m]^q$; M=Fe,Rh,Os interstitial carbides. ^{13}C NMR shifts.	8288	PP
	$M_2(CO)_9$, $M_3(CO)_{12}$; M=Fe-Os. HF/MP2/DFT compared.	8083	PP,DFT
	$H_2M(CO)_4$, M=Fe-Os.	8210	PP
	$OsH_3X(PH_3)_2$; X=Cl,I.	7250	PP
	$[MH_3(PMe_3)_4]^+$; M=Fe-Os	8150	DFT
	$MH_4(PH_3)_3$; M=Fe-Os. Non-classical hydrides of Os due to R.	8613	DFT
	$OsH(Ph)(CO)(PH_3)_2$ + CO.	9384	PP
	MH^+, M=Fe-Os. Compare several PP.	8601	PP
	$M(CO)_5$, M=Fe-Os.	8617	DFT
	$M(CO)_4(C_2H_4)$, M=Fe-Os.	8618	DFT
	Cis-OsO_2F_4.	7227	PP
	MEX_n^q; M=Mo,W,Re,Os; E=N,O; X=F,Cl; n=3-5.	9053	PP
	Os_2Cl_8, $Os_2Cl_8^{2-}$. How short can a M-M bond be?	8984	PP
	Metallacyclophosphazenes $MCl_3[N_3(PH_2)_2]$; M=Ru-Os.	9881	DFT+PP
	OsO_4-catalyzed dihydroxylation of olefins.	7379	PP
	Cp_2M; M=Fe-Os.	7266	PP
	$CpM(CO)^-$ + CH_4; M=Ru,Os.	9860	PP
	Pd and Pt bis(carbene) complexes. PES.	7877	DFT
	Bis(dihydroquinidine)-3,6-pyridazine·OsO_4-catalyzed dihydroxylation of styrene.	10044	PP
	$[M(SiR_3)H_3(PH_3)_3]$; M=Ru,Os.	8075	PP
	$Os(SiR_3)Cl(CO)(PPh_3)_2$; R=F,Cl,OH,Me.	8076	PP
	$[Os(NH_3)_4(OAc)(H_2)]^+$.	7296	PP
	$[Os(NH_3)_4L(\eta^2\text{-}H_2)]^{q+}$: H-D spin-spin coupling.	6771,7100	PP
	$M_3(CO)_9(\mu\text{-}H)_3(\mu_3\text{-}CH)$; M=Ru,Os.	9402	PP
	$[P(CH_2CH_2PH_2)_3M(D)(D_2)]^+$; M=Ru, Os. DQCC.	6782	PP
	$OsCl_2H_2(PPr^i_3)_2$.	8840	PP
	Trans-$[LM(H_2PCH_2CH_2PH_2)_2(\eta^2\text{-}H_2)]^{n+}$; M=Ru,Os; n=1,2; L=H^-, CH_3^-,F^-,CF_3^-, CN^-,Cl^-,Br^-,CO,NCH, NH_3,PH_3. Dihydrogen acidity.	10246	DFT+PP
	$ML_n(L')_{3-n}$ + CH_4; M=Ru,Os; L,L'=PH_3,CO. Competing σ and π approaches found.	9861	DFT+PP
	$OsH_2X_2L_2$; X=Cl-I; L=PH_3.	7917	PP
	$OsH_3(BH_4)(PR_3)_2$.	7427	PP
	$[Os(PR_3)_3"H_5"]^+$.	8841	PP
	$[Os(PR_3)_3H_4]$ and other $[ML_n(H\cdots H)]$.	8843,8844	PP
	$MY_6I_{12}^{2-}$; M=Ru,Os.	6715	MS
	$(CH_3)_2M(\equiv CH)(X)$, $(CH_3)M(=CH_2)_2(X)$, M=Mo,W;Ru,Os; X=Cl,CH_3,CF_3,SiH_3,SiF_3.	7217	PP+DFT
77 Ir	H_2 addition to $Ir(PR_3)_2(CO)X$.	6584–6586	PP

Element	Compounds	Ref.	Method
	MOC, MCO, M=Rh, Ir.	7351	PP
	Ir_3.	7364	PP
	IrC.	9933	PP
	IrN.	9352	PP
	IrO, OIrO, $Ir(O_2)$, $(O_2)IrO_2$, Ir_2O, Ir_2O_2.	7241	PP
	$Ir_2 + H_2$.	7133	PP
	$Ir^+ + CH_4$.	9192	PP
	YIrC, $YIrC_2$.	9452	PP
	MF_6^{2-}; M=Co-Ir. $d-d$ spectrum.	10127	DF/HF
	$M(CO)_6^n$, M=Cr→Fe, Tc→Ru, Hf→Ir. Dissociation energy.	7578,9901	PP
	$CpM(PH_3)(CH_3)^+$ + C-H bonds. M=Rh,Ir.	9855	PP
	$CpM(PH_3)$ + C-H bonds. M=Rh,Ir.	9863	DFT+PP
	CpML + C–H bonds; M=Rh,Ir; L=CH_2,CO,SH_2,PH_3. Singlet-triplet gap.	9865,9866	DFT+PP
	$[Ir(CN)_5]^{3-}$. R/NR.	9067	DFT-DVM
	$CpM(CO) + CH_4$; M=Rh,Ir.	9860	PP
	Trans-$Ir(Cl)(PH_3)_2 + CX_4$; X=F-I.	9864	DFT+PP
	$Ir(trans\text{-}(PH_3)_2)(CO)(i\text{-}Pr_2SiO)$.	10057	PP
	Cis-$[M(CO)_2I_2]^- + CH_3I$.	7890	PP
	$IrXH_2(PR_3)_2$; X=Cl-I; R=H,Me.	7249,7564	PP
	$Ir(PH_3)_2(X) + CH_4$; X=H,Cl.	7315	PP
	$(Cp)ML + CH_4$; M=Rh,Ir; L=CO, SH_2, PH_3.	9857	
	Dito. M = Ru^-,Os^-,Rh,Ir,Pd^+,Pt^+.	9858	PP
	$M(X)(PH_3)_2$ + C-F bonds; M=Rh,Ir; X=CH_3,H,Cl.	9856	DFT+PP
	$IrClH_2(PH_3)_3$.	7980	PP
	$[Ir(H)_2(PR_3)_2]^+$.	7268	PP
	$Ir(H)_2(CO)L$; L=$C_6H_3(CH_2PH_2)_2$. *Cis/trans* isomerization.	8626	DFT+PP
	$[IrH_3(PH_3)Cp]^+$.	8167	PP
	Octahedral L_5M-(CH)=CHR alkenyl complexes. M=Ru,Re,Ir.	7216	PP
78 Pt	PtH, PtH^+, PtH_2.	7522	DF/HF, DK.
	PtH.	10128	DF+CI
	PtH.	7712,7713	DK,PP
	PtH. Mean-field spin-orbit.	8801	PP
	PtH.	9767	DK+SO
	Pt_2.	9158	DK
	PtH, PtH^+, Pt_2, Pt_2H.	10369	PP
	MH; M=La, Hf→Pt.	10219	PP
	PtH, $PtO^{0/+1}$, $PtCH_2^+$. Z_{eff} SO operator.	7990	PP
	PtH_2^+. SO effects.	7645	DK-RASCI
	MH_x^{2-}, MCl_y^{2-}; M=Ni-Pt; x=2,4,6; y=4,6 in crystal field.	8640	DFT
	Solid A_2MH_2; A=Li,Na; M=Pd,Pt.	8645	DFT
	MXe, M=Ni-Pt.	7086	PP
	Pt_n; n=2-12.	10243	PP
	Pt_3, Pt_4.	9478	PP
	M_4, M=Pd,Pt.	7355	PP
	Pt_n^q; n=1-4; q=0,±1.	7739	DFT
	Pt_n; n=2-6,13.	10270	PP
	M_{13}; M=Pd,Pt. SO.	10184	PP

Element	Compounds	Ref.	Method
	Pt_n; n=9-13. $RePt_n$; n=8-12. Models for Pt(100). H_2 dissociation.	9898	DFT
	Pt_nH_m, $Pt_nH_m^-$. Models for on-top H adsorption at platinum electrodes.	10244	DFT+PP
	$Pt_{13}H_n$; $n \leq 20$.	10183	PP
	$ZrPt_3$ cluster.	10158	PP
	MO, MCO; M=Ni-Pt.	7237,7238	DFT
	M_2CO; M=Pd,Pt.	9085	
	CO on Pt(110).	7817	PP
	MO; M=Ni-Pt.	9349	PP
	PtN.	7356,8235	PP
	MXe; M=Ni-Pt.	7086	PP
	$[MX_6]^{2-}$; X=F-Br; M=Ti...Pt. M-X bond energies. Different DFT compared.	7410	DFT
	$[MX_6]^{q-}$; M=Ta→Pt; X=F-Cl; q=0-2. Trends in redox potentials studied.	8757	DFT
	Pt_3Au, PtAu.	7350	PP
	$[Pt_3Fe_3(CO)_{15}]^{n-}$; n=0-2.	9833	DFT
	$M_3 + H_2$; M=Pd,Pt.	7363	PP
	Pt_3/O, Pt_4/O adsorption models.	8422	PP
	$PtSn + H_2$.	7135	PP
	Cu/Pt_9, Ag/Pt_9. Surface models.	9417	PT
	$PtAl$, Pt/Al_9, Pt_4Al_4.	9418	PP
	Mixed-metal clusters with $[Pt_2Au]^{3+}$ and $[Pt_2Hg]^{4+}$ cores.	9995	SR SW
	PtC_n^+; n=1-16. Structures.	8913	DFT/PP
	S/Pt_{12}.	9419	PP
	PtL, ZrL, PtZrL, ZrPtL; L=H,CH_3.	9385	PP
	$PtCN^-$, $PtNC^-$.	7711	PP
	Pt + CO.	9444,9445	PP
	CO adsorption on M; M=Ni-Pt. Relativistic trends.	9121	DFT
	Pt-CO interactions in mordenite zeolites.	10252	DFT
	TM core level shifts upon adsorption on Al_{37} model of Al(100). 'TM'=Ne,K,Cu-Au,Ni-Pt. Covalent interaction.	9122	DFT
	$Pt(CO)_3$, $Pt_3(CO)_6$.	7897	PP
	LM_n chemisorption models. L=HS-, MeS-; n=10,11; M=Pd,Pt.	9660	PP
	$M(CO)_3L$; M=Ni-Pt; L=Co, SiO, ...	7572	PP
	$M_2(\mu\text{-}PR_2)$ core; M=Pd,Pt; PH_3, organic ligands.	8876	DFT+PP
	$M(CO)_4$, M=Ni-Pt.	7575,8209,8617	PP
	$Pt(CO)_4$ as test of ZORA geometry optimization.	10076	DFT
	$M(CO)_4$; M=Ni-Pt. DFT by DPT.	10085	DFT
	$Pt + H_2$.	7459	PP
	H_2 + M, M=Re→Pt.	7899	PP
	$PtCH_2^+$	7993	PP
	$[Pt(CH_3CN)Cl_3]^-$ complex. with alkane and bis(diphenylphosphino)alkane ligands.	9152	PP
	$[Pt_2(\mu\text{-}O_2CCH_3)_4(H_2O)_2]^{2+}$.	9842	SR SW DFT

Element	Compounds	Ref.	Method
	$[(\eta^3\text{-}CH_2CCPh)Pt(PPh_3)_2]^+$.	7870	DFT
	M + C_2H_4; M=Pd,Pt. Ethylene activation.	8924	PP
	$Pt^{0,+1}$ + benzene.	9447	PP
	M + CH_4; M=Re→Pt.	9900	PP
	ML_2 + CH_4; M=Pd,Pt; L=CO,PH_3; L_2=$PH_2CH_2CH_2PH_2$.	9862	PP
	M, M_2 reacting with H_2, CH_4; M=Pd,Pt.	7310	PP
	CH_4 + Pt^+.	7995, 9179	PP
	CH_4 + (eda)$PtCH_3^+$; eda = $H_2N\text{-}CH_2\text{-}CH_2\text{-}NH_2$.	7983	DFT
	CH_4 + Pt photodissociation. Embedded cluster model for surface.	10207, 10208	PP
	Ethyl to ethylene conversion on Pt.	10208	PP
	$PtCH_2^+$.	7993	PP
	CH_4 + $Pt^{0/+/-}$.	7935	PP
	CH_4 + Pt_n; n=1, ...,10.	6618	PP
	Pt_2 + CO.	9449	PP
	$PtCH_2^+$ + NH_3.	6736	PP
	M^+-L; M=Ni,Pt; L=glycine, formate, formamide.	6843	PP
	MO^+ + C-H or C-C bonds. M=Os,Pt.	9620	PP
	CO and O on a Pt(111) slab surface.	6967	PP
	CO adsorption on M(111); M=Ni-Pt.	9234	ZORA
	$[PtCl_2(CO)_2]_2$ dimer: $d^8 - d^8$ interaction.	6754, 9073	PP
	PtI_2.	8058	PP
	$Pt_2(PH_3)_4(\mu\text{-}S)_2$. Complexes with Ga(III), In(III), Tl(I), Pb(II).	9930	PP
	$Tl_2Pt(CN)_4$.	7481	PP
	$[Pt(NH_3)_2]^{2+}$ interaction potential with H_2O.	8988	PP
	$\eta^2\text{-}C_{60}\text{-}Pt(PH_3)_2$.	8414	PP
	^{13}C NMR shifts in M-olefin complexes, M=Cu,Rh,Ag,Pt.	7977	PP
	$C_{59}M$; M=Ir,Pt.	9265	DFT+PP
	$[M(PH_3)_2O_2]$; M=Pd,Pt.	9037	SR DFT
	$[(PH_3)_2PtSe]_2^{n+}$; n=0,2.	6903	PP
	$[Pt(NH_3)_3(adenine)]^{2-}$. Force field determination.	8454	PP
	$Pt(PX_3)_2$; X=H,F. The nature of the Pt-P bond.	7658	PP
	$[M(PH_3)_2(\eta^2\text{-}C_2X_4)]$; M=Ni-Pt; X=H,F,CN. Geometry, bonding.	9078	DFT
	$M(PH_3)_2$ + $BX_2\text{-}BX_2$; M=Pd, Pt; X=H, OH.	9534	PP
	$Pt(PH_3)_2$-catalyzed hydrosilylation of ethene.	9535	PP
	$Pt(PR_3)_2$-catalyzed alkene, alkyne diboration. Pd/Pt?	7308, 7309	PP
	$M(PH_3)_2$ + Si-X bonds; M=Pd,Pt; X=H,Si.	9537	PP
	$PtCl_2(PH_3)_2$ + $SnCl_2$.	9413	PP
	σ-bond activation of $(HO)_2B\text{-}XH_3$ by $M(PH_3)_2$; X=C-Sn; M=Pd,Pt.	9533	PP
	$Pt(H)(PH_3)_2(SnCl_3)(C_2H_4)$. Olefin insertion.	9414	PP
	$MH(\eta^{1,3}\text{-}C_3H_5)(PH_3)$; M=Pd,Pt.	9539	PP
	Diimine-M(II) complexes (M=Ni-Pt), and their zirconocene complexes in olefin polymerization.	8999	PP
	$Pt(PR_3)_2$ + H_2.	8853	PP
	PtL_2 + H–OCH_3. L_2=$(CO)_2$, $(PH_3)_2$, diphosphine.	9859	PP
	$PtH(SiH_3)(PH_3)$ + C_2H_2.	9878	PP

Element	Compounds	Ref.	Method
	$PtH_3(PH_3)_2^+$. Dihydrogen complex.	7918	PP
	$CpM(CO)^+ + CH_4$; M=Pd,Pt.	9860	PP
	$[M(PH_3)_2]_nC_{60}$; M=Pd,Pt; n=1,2,6.	6982	PP
	$M(PH_3)_2X_2$; M=Ni-Pt; X_2=O_2,C_2H_2,C_2H_4.	8618	DFT
	Pt(II)(OOH) complexes.	7659	PP
	MM'$(PH_3)_4$; M,M'=Pd,Pt. $d^{10} - d^{10}$.	9538	PP
	A Pt_2(II,III) bridged model system $[Pt_2(\mu\text{-}C_6F_5)_2(CF_3)_4]^-$.	10055	SR DFT SW
	$Pt_2(dta)_4X_2$; X=Br,I. 'dta'=$CH_3CS_2^-$.	9409	PP
	Peierls distortions in the chain.		
	Dimers of M$(dmit)_2$; M=Ni-Pt, 'dmit^{2-}' = 2-thioxo-1,3-dithiole-4,5-dithiolato.	9433	DFT
	$Pt_2[NHCHN(C(CH_2)(CH_3))]_4$. $d^8 - d^8$.	9039	PP,DFT
	$[Pt_2Cl_2(CO)_4]$, $[Pt_2Cl_4(CO)_2]^{2-}$. $d^9 - d^9$ bond.	9877	PP
	MM2 force field derived for Pt(II) square complexes.	7319	PP
	Ethylene polymerization catalyzed by diimine-M(II); M=Ni-Pt.	9002	PP
	$Pt(PH_3)_2$(R), R=olefin (C_2H_4, C_8H_{10}, ..., $C_{11}H_{16}$).	10041	PP
	$(X_3P)_2Pt$=PR phosphinidenes.	6909	PP
	$Pt(P(t\text{-}Bu)_3)_2 + H_2$, Diels-Alder reaction of acrolein + isoprene, etc.	9896	PP
	$(C_2H_4)MCl_x(NH_3)_{3-x}$; M=Ni-Pt; x=1-3.	9844	PP
	$M[(CHNH)_2]R^+$ + ethene; M=Ni-Pt; R=Me,Et.	9845	PP
	$[Pt(NH_3)_2L_2]^{2+}$; L=Cl^-, H_2O.	7126	PP
	'Carboplatin' versus 'cisplatin'.	9994	PP
	Trans-$[(CH_3NH_2)_2PtCl_2]$ + adenine, thymine.	7125	PP
	$M_3(CO)_6^{2-}$ Cini clusters (M=Ni,Pt).	6905	PP
	HCN synthesis from CH_4+NH_3 on Pt^+.	7456	PP
79 Au	Au_2	6850	DFT
	M_2; M=Cu-Au.	10090	DV DFT
	M_2; M=Cu-Au, AuH, AuCl.	8868	DFT
	M_2, MH, MCl; M=Cu-Au. R/NR.	9892	SR DFT
	Various functionals, finite nuclei compared.		
	CuAg, CuAu, AgAu. Electric properties.	8324	PT
	Au_3	6723	MS
	Au_n; n=2-6	7048,7049	PP
	M_n; n=5,7; M,M'=Cu-Au. g-factors, hfs at ZORA level.	10078	DFT
	Au_{13}.	8560	DFT
	Au_n; $n \leq 75$.	7812	PP
	Au_n; n=2,6,55. $AuPR_3$, $MeAuPR_3$. Naked and clad $[Au_6]^{m+}$.	7927	DFT
	Au_n; $n \leq 147$.	7928,8482	DFT
	Octahedral M_6, M=Ag,Au.	6714	MS
	Au_n^q; n=1-4; q=-1,0,+1.	9669	PP
	R/NR orbital energies for M_6, M=Cu-Au.	6589	DFT
	$(Au)_\infty$: infinite 1D chain.	9087	DFT+PP
	Au_8 on MgO surface. Catalyst for CO oxidation.	9550	PP
	$(Au_n^+)CH_3OH$; $n \leq 15$.	9463	DFT+PP
	Car-Parrinello study of adsorption.		
	$Au_3(PH_3)_4L_n$; n=0-3; L=-$InCl_2H_2O$.	7796	DFT

Element	Compounds	Ref.	Method
	Also Au_3^q, $Au_3(PH_3)_4^q$; q=0,+1. $Au_3(PH_3)_3^+$.		
	MM'; M=Rh, ...Au	7962,7963	PP
	Au_6^q; q=0-4. Au_6X^q; X=B,C,N. $[(LAu)_nX]^q$; n=4-6.	7930	DFT
	$Au_{12}Pd$	6720	MS
	M_nAu; M=Na,Cs; $n \leq 9$.	7998	DFT
	AuH.	9261	DK
	AuH.	8243	DK CC
	MH; M=Cu-Au. Dipole moments.	8323	PT
	MH; M=Cu-Au. Dipole moments.	8325,8333	DK
	MH; M=Cu-Au. Comparison between methods	7257	PP
	MH; M=Cu-Au. Comparisons at MP2 level.	7747	DPT,PT
	MH; M=Ag,Au. Test new method.	9015	RESC
	MH, MCl; M=Ag,Au. Test new method.	9016	DFT+RESC
	M_2, MH; M=Ag,Au. Test two-electron terms.	9158	DK
	Au_2, AuH as tests of the ZORA approximation.	10073	DFT
	MM', MX; M=Cu-Au, X=H,F,Cl. ZORA/PT with DFT.	10087	DFT
	MH; M=Ag,Au, Au_2 as tests of DFT by DPT.	10083	DFT
	Au_2, AuH. Spin-orbit effects.	8595	PP
	Au_2, AuH. Spin-orbit effects via ZORA.	10077	DFT
	Au_2,AuH,AuCl.	9037	SR DFT
	AuF, AuF^+, AuF_2, Au_2F_2.	9643,9644	PP
	MF; M=Cu-Au.	8551	DF+MP2
	MF_n^-; M=Cu-E111; n=2,4,6.	9677	PP
	MF; M=Cu-Au.	8099	DK
	AuCl.	6781,9633	PP
	AuX; X=F-I.	7530	DF
	Au_2Cl_6. PES.	8125	DSW
	MI, M_2I^+, M_3I^{2+}, M_4I^{3+}; $[I(MCl)_m]^-$; m=1-4;	6647	PP
	M=Cu-Au.		
	AuI_n^-; n=2,4	9897	PP
	$[(AuCl_3)_2(\mu\text{-}Cl)]^-$.	9614	PP
	Occurs in room-temperature molten salt.		
	Diatomic CsAu.	9573	DF/HF
	SiM; M=Cu-Au. All ground states $^2\Sigma$. $SiCu^{\pm}$.	10037,10038	DK
	$[XMX]^{3-}$; M=Cu-Au; X=O-Se in crystal field.	8636,8637	DFT
	BM; M=Cu-Au.	6839	DK
	AlM; M=Cu-Au. Electric properties.	10054	DK
	AuX^+; X = Be,Mg, C, Si. Au≡C^+ triple bond found.	6836	DK
	$RgAu^+$, $RgAuRg^+$; Rg=He-Xe predicted.	9303	PP
	$ArAu^+$, $XeAu^+$ handled with polarization and dispersion.	9373	
	Au_2O, MO_n; n=1-3; M=Ag,Au. AuO_2 observed.	7242	PP
	Au≡C^+. Do other Au≡L exist?	9316	PP
	SAu_3^+, $S(AuPH_3)^+$. $d^{10} - d^{10}$.	9305	PP
	$(XAuPH_3)_2$; X=H,F-I,CH_3,-CCH,CN,-SCH_3. $d^{10} - d^{10}$.	9308,9311	PP
		9309	
	$MeAuPR_3$; R=H,Me,Ph.	7929	DFT
	$ClAuPH_3$, $ClAuPH_2Ph$, $ClAuPPh_3$. Eigenvalue spectrum.	8571	SR SW
	$(ClAuPH_3)_n$ isomers, n=2,4.	9312	PP
	$H_2C[P(Ph)_2AuX]_2$, $HC[P(Ph)_2AuX]_3$; X=Cl,I. $d^{10} - d^{10}$.	9869	PP

Element	Compounds	Ref.	Method
	$H_3PS[Au(PH_3)_n]^{n+}$; n=1-3. $H_2P(S)S[Au(PH_3)]_2^+$. $d^{10}-d^{10}$.	9295	PP
	$[(PR_3)_2M]^+$, $[PR_3MCl]$; M=Ag,Au; R=H,Me.	7034	DFT
	Au(I)...Au(III) interactions modelled by $[S(AuPH_3)_n(AuH_3)_{3-n}]$.	7108	DFT
	M_2Se, M_2I^+, M=Ag,Au.	6648	PP
	$H_3PAuC{\equiv}CAuPH_3$ complex with $CHCl_3$	7650	PP
	MCO; M=Cu-Au.	9635	PP
	$M(CO)^+$; M=Ag,Au.	7378	PP
	MCO^+; M=Cu-Au.	8745	PP
	$AuCO^+$. Accurate.	7382	PP
	H_2 on M(111); M=Ni,Cu,Pt,Au. 'Why gold is the noblest of all metals'. Relativity not mentioned.	7953	PP+DFT
	Adsorption of M on cluster models of NaCl(100); M=Cu-Au.	8883	PP
	CO on M(111); M=Ni,Cu,Pd,Ag,Pt,Au; Ru(0001),Cu_3Pt. Simple model for d-band hybridization proposed.	7952	PP+DFT
	NO_2 on Au atom, Au clusters.	8722	DFT+PP
	ClM(CO), M=Cu-Au.	6687	PP
	$M(CO)_2^+$, $[M(CO)_2F_2]^-$; M=Cu-Au. 'Nonclassical' metal carbonyls.	8746	PP
	$[M(CO)_n]^{z+}$; M^{z+}=Cu^+-Au^+, Zn^{2+}-Hg^{2+}; n=1-6.	8748	PP
	$M(CO)_n^+$; MCN, $M(CN)_2^-$; M=Ag,Au; n=1-3.	10095	PP
	$[Au(CN)_2]^-$ to $[Tl(CN)_2]^+$, $[Au(CO)_2]^+$ to $[Tl(CO)_2]^{3+}$. DFT, MP2, CCSD(T).	8211	PP
	Bimetallic clusters: $[M_4\{Fe(CO)_4\}_4]^{4-}$; M=Cu-Au.	6627	DFT
	MR; M=Cu-Au; R=Me,Ph.	6688	PP
	MBH_4; M=Cu-Au.	9000	PP
	Au speciation in aqueous solution.	10001	PP
	Decomposition of Au(I) compounds.	10003	PP
	AuSH, $Au(SH)_2^-$ + H_2S, H_2O	9049	PP
	Cyclic $[Se_nAu_2]^{2-}$; n=5,6: $d^{10}-d^{10}$.	6769	PP
	$(M_2S)_n$; n=1,2; M=Ag,Au: $d^{10}-d^{10}$.	6776	PP
	$[XAuPH_3]_2$; X=H,Cl. $d^{10}-d^{10}$.	9487	PP
	Pt_3Au, PtAu.	7350	PP
	Solid MCl; M=Ag,Au. $d^{10}-d^{10}$.	7485	PP
	$M{=}CH_2^+$, $M\text{-}CH_3^+$; M=Cu-Au.	8059	PP
	MCH_2^+; M=La,...Au.	8124	PP
	MCH_2^+; M=Fe,...Au.	7456	PP
	MCH_2^+; M=Ni,Pd,Ir→Au. HCN synthesis from methane and ammonia.	7987	DFT
	Au+ethylene interaction.	8887	PP
	ClM=M'R_2; M=Cu-Au; M'=C-Ge. R/NR for Au.	6991	PP
	MCH_3^+; M=Sc-Cu,La,Hf-Au.	8044	PP
	C_6H_6 + M^+; M=Cu-Au.	7383	PP
	C_2H_4 + M^+; M=Cu-Au.	8012	PP
	H_2O + Au^+.	8061	PP
	$M^+(H_2O)_n$; n=1-4; M=Cu-Au.	7673	PP
	Au_n^+; n=1-15 + CH_3OH.	9463	PP
	$[Me_3P\text{-}Au]^+$ + alkyne + alcohol.	9953	PP
	$[E(AuPH_3)_4]^+$; E=N-As. $d^{10}-d^{10}$.	8615	PP

Element	Compounds	Ref.	Method
	$X(AuPH_3)_n^{m+}$; X=C,N,O,P,S; n=1-6. $[HC(AuPH_3)_4]^+$. $d^{10} - d^{10}$.	9317	PP
	$[OAu_3]^+$, $[O(AuPH_3)_3]^+$, dimers.	7239	DFT
	$[CH_2(PH_2AuPH_2)_2CH_2]^{2+}$.	7686	PP
	$[M_2(H_2PCH_2SH)_2]^{2+}$; M=Cu-Au.	7687	PP
	Rings $[M_2(PH_2CH_2PH_2)_2]^{2+}$, $[M_2(NHCHNH)_2]$, $[M_2(SCHS)_2]$, $[M_2X_4]^{2-}$; M=Cu-Au; X=Cl-I.		
	$[Au_2(PH_2CH_2PH_2)_2]Cl_2$. $[Au_2Te_4]^{2-}$. $d^{10} - d^{10}$.	9310	PP
	$Au_2X_2C_2H_2(PH_2)_2$; X=Cl-I. *Cis* has $d^{10} - d^{10}$. Photochemistry of cis-to-trans conversion.	9638	PP
	Cl_nAuSMe_2; n=1,3. Inversion at sulfur.	10009	PP
	$[Cp_2Ti(C{\equiv}CH)_2]$Au-R.	8417	DFT+PP
	$[Cl_2Ti(C{\equiv}CH)_2]MCH_3$ 'tweezers'; M=Cu-Au.	8450	PP
	(Et_3P)Au(2-Thiouracil).	9835	PP
	$AuPt^-$, Au_2, $AuHg^+$.	10199	PP
	$AuPt_n + H_2$; n=1,2.	7306	PP
	$AuPt_2$, Au_2Pt + ethene.	7305	PP
	$[(AuPH_3)_6Pt(PH_3)]^{2+} + H_2$. Model for dihydrogen activation.	10245	DFT+PP
	$Au(C_2H_4)$.	8887	PP
	$[Au(III)(C_6H_4S_2)_2]^-$. Aromatic Au(III) dithiolene.	9592	PP
	Au^+-L; L=H_2O, CO, NH_3,C_2H_4,...	8010,8060,8061	PP
		9619	PP
		9621	PP
	$ClMPH_3$, MPH_3^+; M=Cu-Au.	8357	DFT+PP
	M^+-L; M=Cu-Au; L=adenine, guanine.	7087	PP
	M^+-L; M=Cu,Au; L=glycine, formate, formamide.	6843	PP
	M^+-L; M=Cu-Au; L=C_2H_4, N_2, HCN, C_2H_2, N_2O, FCN, HCNO, HN_3, HCCF, CH_2N_2, CH_3CN, C_2F_2, FCNO, CH_3CNO	6844	PP
	$[M_2(\mu\text{-}Y)(\mu\text{-}XR)L_4]$, $[M_2(\mu\text{-}XR)_2L_4]$; M=Rh→Pd, Ir→Au; X=O-Te; Y=Cl,S: $d^8 - d^8$.	6755,6756	PP
	$[Au(\overline{CNHCH=CHN}\ H)_2Cl_2]^+$, $[Au(\overline{CNHCH=CHN}\ H)_2]^+$. carbenes.	9367	PP
	M_5Ph_5; M=Cu,Au.	6897	DFT
	Au_9-SCH_3.	6872	PP
	Au_{12}/H_2S, $HSCH_3$.	9662	PP
	M_{16}/SH, SCH_3; M=Ag,Au.	9665	PP
	$Au_{38}(SCH_3)_{24}$. Capacitance.	7944	PP
80 Hg	Hg_2.	7476,7700,9642	PP
		7340,9879,9880	PP
	Hg_2 from interaction potentials.	8497	DK
	Hg_2, Hg_2^+, Hg_3.	6854	DFT
	Hg_n.	7477	PP
	Hg_n.	9765	SR DFT
	M_2; M=Zn-Hg.	10296	PP
	M_n, $n \leq 6$, M=Zn-Hg.	7703,9587	QMC+PP
	M_2^{2+}, M=Zn-Hg. Their compounds.	8308	PP
	Hg_2^{2+}. Interpretation of relativistic effects.	9630	DFT

Element	Compounds	Ref.	Method
	HgX_2; X=Cl-I. ^{199}Hg NMR shifts.	9021	PT
	MX,MX_2,M_2X_2; M=Zn-Hg; X=F-I. Molecules and solids.	8644	DFT
	Hg_2^{2+}, Hg_2L_2; L=F-I. Molecules and solids.	8633,8638,8643	DFT
	Hg_n^{2+}; n=2,3. Complexes with Cl, C_6H_6.	10047	PP
	Hg_n + $H_2/O_2/F_2$. Dissociation models for surface of liquid mercury. Potential functions.	9663,9664	PP
	$AuHg^+$.	10199	PP
	HgCd.	6947	PP
	HgH.	6638	PP
	HgH, HgH^+.	7972,8983	PP
	MH; M=La→Hg.	7131	PP
	MH^+, MH_2; M=Zn-Hg. Vibrational spectra.	7878	PP
	LiHg.	7835,7906,7907	DK
	NaHg.	7905	DK
	CsHg. Green bands.	9272,9273	DK
	HgO.	8064,8065	DF
	MS; M=Zn-Hg. Electric properties.	9364	DK
	HgX_2; X=Cl,CN.	6615	PP
	HgX, HgX_2, Hg_2X_2; X=H,F,Cl,CH_3,CF_3. Hg_2^q; q=0,+1,+2.	9636	PP
	MR_2; M=Zn-Hg; R=Me,Ph.	6688	PP
	LHgL'; L=Cl-I,Me,CN. ^{199}Hg NMR shifts using ZORA.	10222	DFT
	$Hg(CF{=}CF_2)_2$.	6810	PP
	Photodecomposition of Hg methyl complexes.	10004	PP
	HgI_2.	8058	PP
	HgF_4.	8305,8306	PP
	HgX_n; n=2,4; X=F,Cl.	8690	PP
	MO_4^q; M=Ir-Hg. Extreme oxidation states ($d^{0/2/4}$). HF only.	7433	PP
	HgX_2, $(HgX_2)_2$; X=H,F-I. R/NR.	8307,8309	PP
	Solid MF_2; M=Cd,Hg.	8309	PP
	HgL_2; L=F,Cl,Oh,Sh,CN. $HgCl_n^{2-n}$; n=1-4. $Hg_3S_2(SH)_2$ model for cinnabar. Hydration.	10005	PP
	$MeHg^+$, Me_2Hg, MeHgX (X=Cl-I), $MeHg(PH_3)^+$, $[MeHg(PH_3)_3]^+$.	6816–6818	PP
	RHg, RHgH; R=Me, CH_2CH-, MeO(CO)(MeC)CH-.	9018	PP
	$CH_n(HgX)_{4-n}$; X=Cl,CN; n=0-4. RHgH; R=Me, Et,... . ^{13}C and ^1H NMR shifts.	8297	DFT+PP
	TM carbonyl ^{13}C NMR shifts; TM=Hf-Hg.	10222	
	Mercury sulfides.	9843	
	Solid $2HgS{\cdot}SnBr_2$	9481	PP
	$(HgPMe)_n$, n=4-6,8,12	6600	PP
	$M(CO)_2^{2+}$, $[M(CO)_2F_2]$; M=Zn-Hg	8746	PP
	$[FeHgCp_2]^{2+}$, $[FeCp(C_5H_4)Hg]^+$ ferrocene derivatives.	8870	DFT
	H_2→ 2H on Hg surface.	9661	PP
	M^{2+}-L; M=Cd-Hg; L=adenine, guanine	7087	PP
	M^+-L; M=Cd,Hg; L=glycine, formate, formamide	6843	PP
	XH_4 + $M(^3P)$ → $HMXH_3$ (X=C,Si; M=Zn-Hg)	6654	PP
	Hydrated M^{2+} + adenine, thymine base pairs; M=Zn-Hg	9809,9810	PP
	Hg^* ($^3P_1$) + H_2, CH_4, C_3H_8, SiH_4	9752	PP
	$FHgX$ + CH_4; X = NH_2, NO_2, N_3,...	7326,7329	PP

Element	Compounds	Ref.	Method
81 Tl	Tl_2.	8363	PP
	Tl_2, TlH. Spin-orbit effects	8595	PP
	TlH.	8364,9348	PP
		9344,9590	
	TlH, TlH_3.	7956	PP
	MH, MH_3, M_2H_6; M=In,Tl	8084	PP
	M_2H_2; M=B-Tl	10012	PP
	TlCl	8629	PP
	TlF. *PT*-odd interactions.	8552,9161	DF
		9330	
	TlX; X=F-I	7530	DF/HF
	TlH, TlX; X=F,I. Spin-orbit effects via ZORA.	10077	DFT
	TlX, TlX_3; X=F-I.	9641	PP
	MX_3, MH_2X; X=F-I; M=B-Tl.	7751	PP
	TlX_2^+, $TlX_2^+ \cdot 4H_2O$; X=Cl,CN.	6615	PP
	$[Au(CN)_2]^-$ to $[Tl(CN)_2]^+$,	8211	PP
	$[Au(CO)_2]^+$ to $[Tl(CO)_2]^{3+}$. DFT, MP2, CCSD(T).		
	TlAr.	8598	PP
	MO_2^-; M=In,Tl.	6678	PP
	M_2O_2; M=Al-Tl.	6703	PP
	M_2O_3; M=Ga-Tl.	6704	PP
	$Tl_2E_2^{2-}$; E=Se,Te.	7017	PP
	$TlMTe_3^{3-}$.	7018	PP
	TlCp, $TlCp_2^-$.	6706	PP
	MCp, $(MCp)_2$, MCp_3, $MCp^{\pm}$, MH, $(MH)_2$.	9314	PP
	Evidence for a Tl(I)-Tl(I) attraction.		
	$Tl_2Pt(CN)_4$.	7481	PP
	$TlN(SiMe_3)_2$.	7926	PP
	$H_3M\text{-}EH_3$; M=B-Tl. Uses a molecular EH_3 effective potential. E=N-As.	9659	PP
	Tl^+ in alkali halides. Stokes shifts. Lifetimes.	6924,9407	PP
82 Pb	Pb_2.	7389,10103	PP
	Pb_2^-.	7360	PP
	M_5^{2-}; M=Sn,Pb.	10048	PP
	Pb_n; n=3-14.	8960	PP
	$Pb_9^{3-/4-}$.	7114	PP
	Na_6M, M=Mg,Pb. Pb inside, Na outside.	6626	DFT
	MH_2, MH_4; M=Si-Pb, MO; M=Ge-Pb.	6813	PP
	MH_2; M=C-Pb. $^1A_1$ and $^3B_1$. SO.	8854	PP
	MH_3^-,MH_4,MH_5^-; M=Si-Pb.	8941	PP
	MH_4; M=C-Pb.	9831	PP
	MH_4; M=Ge-Pb. Electron scattering, elastic and inelastic.	6927,6928	PP
	MH_4; M=C-Pb. Rotational excitation by electron impact.	10089	AE,PP
	MO, MH_4, MCl_4; M=C-Pb. R/NR.	10166	DFT
	$Pb_nH_m^{0/+1}$.	7957	PP
	M_4H_4; M=C-Pb.	9814	PP
	PbH_2, PbH_4.	7956	PP
	Aromatic or polyhedral compounds with Ge, Sn, Pb skeletons.	9008,9009	PP
		9010	

Element	Compounds	Ref.	Method
	EM_6; E=C-Pb; M=Li-Cs. Hypermetallation is ubiquitous.	8821,10138	PP
	M_nPb_m; M=Li,Na; m=1,4.	8958,8959	PP
	MH_4; M=Sn,Pb. Low-energy electron scattering.	6928	PP
	MH_4, MH_3Me; M=Ge-Pb.	7984	PP
	MH_5^-; M=Si-Pb.	8941	PP
	MMe_2Cl_2; M=C-Pb. Bent's rule for bond angles.	8208	PP
	$M_3H_3^+$; M=C-Pb.	8178	PP
	PbBr.	6900	PP
	PbI.	6901	PP
	MF_2; M=Ge-Pb.	7347	PP
	PbI_2.	8058	PP
	Solid $Pb(N_3)_2$.	10294	PP
	MX_3^+, MH_2X^+; M=C-Pb; X=F-I.	7751	PP
	MO; M=Ge-Pb.	7480	DF,PP,PT
	MO, MS; M=Si-Pb. Electric properties.	8321	PT
	MO, MS; M=Si-Pb. Electric properties.	8332	DK
	MX_2, MX_4; M=C-Pb; X=F-I.	7633	PP+DFT/HF
	LSDA, BLYP, B3LYP functionals compared.		
	PbX; X=O-Te. R/NR.	7530	DF
	PbO. R/NR.	8855	DF
	PbO. Dipole moment.	7480	PP
	PbO. Test of new PP.	10213	PP
	PbO, PbX_2.	7530	DF,ESC
	PbX; X=O,Te. Spin-orbit effects via ZORA.	10077	DFT
	Solid PbS.	8902	PP
	MX_2, MX_2^+; M=Ge-Pb.	6666	PP
	Me_3PbX; X=Cl-I, -OMe, -SMe, -SeMe, $-NEt_2$.	9420	DFT
	PbX_4; X=Cl-I. ^{207}Pb NMR shifts.		
	Pb_nO_m; n=1-4; m=1-4.	7207	PP
	PbR_nX_{4-n}, PbR_nX_{2-n}. Why org. Pb(IV), inorg. Pb(II)?	8303	PP
	MH_3-Cl; M=C-Pb. 'Charge-shift bonding'.	9740	PP
	M_2H_6; M=Si-Pb. Core polarization important.	9056	PP
	$M_2E_3^{2-}$; M=Sn,Pb; E=S-Te.	7018	PP
	M_mPb_n; M=Li-K; m=2-7; n=1,4.	6660,7154	PP
	H_2MO, Me_2MO; M=C-Pb.	8262	PP
	$H_2C{=}MH_2$; M=C-Pb.	8152	DFT
	$H_2M{=}MH_2$; M=C-Pb.	8397	PP
	$H_2M{=}MH_2$, H_2MO; M=Si-Pb.	8263	PP
	Coordination of stannocene, plumbocene.	6705	PP
	Group 14 metalloles: $C_4H_4MH_2$, $C_4H_4MH^{\pm}$, $C_4H_4M^{2-}$, ...	7847	PP
	M-C bonds; M=Ge-Pb. H_3M-Y; Y=H, A, ... $ABCDH_3$.	6845	PP
	p-Toluene-XY_3^+ complexes; X=C-Pb; Y=H,Cl,Me.	6841	PP
	H_3M'-MH_3^+, H_3M-Y bond energies, M,M'=C-Pb. 68 ligands, Y.	6842	PP
	$(Me_2NCH_2)_2$ adducts of MCp_2, M=Sn,Pb	6705	PP
	Mono- and bis-amidinate ($[HNCHNH]^-$) complexes of Si-Pb. Valence isoelectronic ligands studied.	9605	PP
	Diphosphanylmethanide ($[R_2PCHPR_2]^-$) M(II) complexes; M=Si-Pb.	9606	PP

Element	Compounds	Ref.	Method
	HMOOH, MeMOOH isomers; M=C-Pb. Shift from M(IV) to M(II).	9396,9397	PP
83 Bi	Bi_2.	7388,10103	PP
	Bi_2. Spin-orbit effects via ZORA.	10077	DFT
	M_2; M=Tl,Pb,Bi.	6852	DFT
	M_4, M_6; M=P-Bi. Benzene analogues, prismanes etc.	8405	PP
	M_n^-; M=Sb,Bi.	7814,8281	DFT
	Bi_5^{3+}.	8092	PP
	M_5^{3+}; M=Sb,Bi.	10048	PP
	Bond lengths for many small inorganic molecules, up to BiH. A test on the authors' PP.	7966	PP+DFT
	BiH.	6634,7461	PP
	MH; M=Tl→Bi.	10213	PP
	MH_3; M=As-Bi.	7051	PP
	MH_4^-, MF_4^-; M=P-Bi.	8942	PP
	MH_5; M=P-Bi.	8943	PP
	MF_5, MH_6^-, MF_6^-, MH_7^-, MF_7^-; M=P-Bi.	8944	PP
	BiF.	6636	PP
	BiI.	6635	PP
	BiN.	6640,6642	PP
		6633	
	BiX; X=N-Sb.	7530	DF/HF
	BiO.	6641	PP
	BiS.	8682	PP
	R-Bi=Bi-R.	9983	PP
	R-M=M-R; M=As-Bi.	7286	PP
	MF_3; M=N-Bi.	9637	PP
	MX_3; M=N-Bi; X=F-I.	9640	PP
	MF_7^{2-}; M=As-Bi.	7498	PP
	$(RhBi_7)Br$. $5c-4e$ bonding.	10248	PP
	MMe_5; M=Sb,Bi.	7924	PP
	BiOH, HBiO.	8341	PP
	PMH_2; M=As-Bi.	8760	PP
	$Bi_3O_4^+$, $Bi_5O_7^+$.	8376	PP
	$[H_2E\text{-}EH_2]_2$; E=As-Bi. Chain fragments.	8398	PP
	Bi_2H_4. $(C_4H_4Bi)_2$. Chain fragments. HF-level.	8711	PP
	$[Bi_4Co_9(CO)_8(\mu\text{-}CO)_8]$.	10366	DFT
	$H_3M{=}CH_2$; M=N-Bi. Their reactions.	9014	PP
	Test of Troullier-Martins (1991) PP on R_e, ω, and D_e of a large number of small molecules, $Z \leq 83$.	7175	PP+DFT
84 Po	M_3; M=Se-Po	6789	PP
	HE; E=O-Po.	9257	DF/HF
	H_2E; E=O-Po.	9256	DF/HF
	M_2H_2; M=Tl→Po.	7957	PP
	$[HE\text{-}EH]_2$; E=Se-Po. Chain fragments.	8398	PP
	PNC for chiral molecules HEEH; E=O-Po. HTeOH.	8553	DF.
	EF_6^{2-}; E=Se-Po. Structure.	8302	PP,DPT
	CuX, Cu_2X; X=O-Po.	8762	PP
	PoX; X=C-Sn.	7530	DF/HF

Element	Compounds	Ref.	Method
85 At	X_2; X=F-At. DF to DF+CCSD(T).	10122	
	HX; X=F-At. Up to CCSD(T). R/NR.	10130	DF+corr
	MH; M=Tl→At.	7462,9651	PP
	X_2, XH; X=F-At.	7473	PP
	HX, HX^+; X=F-At.	9651	PP
	AtX; X=B-In.	7530	DF/HF
	$(HX)_2$; X=F-At.	7085	PP
	AtN_3.	8390	PP
	CH_3X, CX_4; X=Br-At.	7957	PP
	XF_3; X=Cl-At.	9634	PP
	XF_6^-; X=Cl-At. Structure.	8302	PP,DPT
	Me_2SeX_2; X=F-At.	8252	DFT
86 Rn	Rn_2	7954	PP
	Xe_2, XeRn, Rn_2.	9486	PP
	$FeRg^+$; Rg=Ar-Rn.	7994	PP
	$CoRg^+$; Rg=Ar-Rn.	7992	PP
	RgX_n; Rg=Kr,Xe,Rn; X=F,Cl. Molecules and solids.	8641	DFT
	RgF_6; Rg=Ar-Rn. Structure.	8302	PP,DPT
	$MgRn^+$.	7232	PP
	$Rn{\cdot}H_2O$ complex.	8594	PP
87 Fr	MF; M=K-Fr. Electric properties.	8901	PT/DK
88 Ra	$M^{2+}(H_2O)_n$; M=Mg-Ra; n=1-6	7836	PP
90 Th	Th_2^{179+} model.	7746	DPT
	ThH_n; n=1-4.	9806	DFT
	ThO.	10181,10182	DF
	ThO	7804,8486	PP
	ThO^+	7275	PP
	NThO.	10350	DFT+PP
	CThO. Bent triplet.	10352	DFT
	ThN, ThN_2, ThN_4, Th_2N_2.	8505	DFT
	ThF_4. Assumed R 215 pm.	8786	DF
	$M(C_8H_8)_2$; M=Ce,Th	7478,7479	PP
	$Th(Cp)_3$. R $6d^1$, NR $5f^1$ ground state.	8255	DV DFT
	$H+MCl_3$; M=Hf,Th. Bond energy. SR/NR.	10204	DFT
	Cp_3ThOCH_3. PES.	7913	DFT
	$Cl_2\overline{Th(CH_2PMeCH_2)}$	7451	PP
	$Th(S_2PMe_2)_4$.	8148	DFT
91 Pa	PaX_6^{2-};X=F-I, $5f^1$. Optical transitions.	8253	DFT
	MX_6^-; M=Nb,Ta,Pa,Db; X=F,Br.	9196	DV DFT
	$Pa(COT)_2$ $5f^1$.	8255	DV DFT
92 U	UH_n; n=1-4, U_2H_2, U_2H_4.	9807	DFT
	UF^{n+}; n=1-3.	9615	PP
	UO_2^+, UO_2^{2+}.	7273,7274	PP
	UO_2^{2+} excited states.	10340,10354	PP
	UO_2^{2+}, $HOUO^{2+}$, $U(OH)_2^{2+}$.	10066	PP
	$UO_2^{2+}{\cdot}L_n$; L=F^--Cl^-,OH^-,H_2O. Equatorial coordination.	10022	PP
	UO_2^{2+} with coordination of H_2O, OH^-. Simulates strongly alkaline solutions. Evidence for $[UO_2(OH)_4]^{2-}$.	10152	PP
	ThO_2, PaO_2^+, UO_2^{2+}. Bonding and bending.	7529	DF

Element		Compounds	Ref.	Method
		UN, UN_2, U_2N_3, U_2N_2.	8505	DFT
		UN, UO, NUO, NUO^+, NUO_2, $OU(\mu\text{-}N)_2UO$.	8506	DFT
		CUO, CUO^-, OUCCO, $(\eta^2\text{-}C_2)UO_2$, $U(CO)_n$; n=1-6.	10351	DFT
		NUO^+ isoelectronics, UO_3, UO_6^{6-}, UF_6,		
		$(OUO)^{2+}L_n$; L=CO_3^{2-}, NO_3^-,n=3; L=F^-, n=2-6.	9307	PP
		NUO, NUO^+.	10350	DFT+PP
		Uranyl nitrate complexes.	9082	DVM DFT
		NUO^+, NUS^+.	7991	PP
		MN_2; M=Mo,U.	7065	DFT
		Cluster models for solid UC.	8499	DV DFT
		$[UO_2X_4]^{2-}$; X=OH,F,Cl.	9608,9609	DFT+PP
		Both *trans*- and *cis*-uranyls found.		
		UF_4. PES.	8990	DFT
		UCl_4	7925	PP
		UF_5.	9100	DVM DFT
		UF_6.	9104	DVM DFT
		UF_6.	9169	SR SW
		$An(C_6H_6)_2$; An=Th,U.	8047	PP
		UF_6. Assumed R 199.9 pm.	8787	DF
		UF_6^q, q=0,-1. R/NR.	7415	DF
		$M(CO)_6$; M=Cr,W,U,Sg.	9030	PP
		$U@C_{28}$.	7151	PP
		$An@C_{28}$; An=Pa,U.	10341	PP
		Cp_3AnL; An=Th,U; L=Me, BH_4.	7452	PP
		OPR_3 complexes of UO_2^{2+}, $UO_2(NO_3)_2$. R=H,Me,Ph.	8085	PP
		$U(C_8H_8)_2$. Excited states.	8687	PP
		Lanthanocenes are $4f^n\pi^3$, actinocenes $5f^{n-1}\pi^4$.		
		Bispentalene complexes $[An(C_8H_6)_2]$; An=Th,U.	7247	DFT
		$[(NH_2)_3(NH_3)U]_2(N_2)$. Actinide dinitrogen complex.	8256	DFT
		Mainly U→N_2 π^* backbonding.		
93	Np	$An(NH_2)_3$; An=U,Np.	7978	PP
		PaX_6^{2-}, UX_6^-; X=F-I, NpF_6. $5f^1$ optical spectra.	8254	DV DFT
94	Pu	Pu_2.	6702	PP,DFT
		AnH_3; An=Th,U,Pu. Orbital energies.	9603	DV DFT
		AnF_6; An=U→Pu.	7979,9609	DFT+PP
		$(AnF_6)_n$; n=1,2; An=U,Pu.	7799	PP
		PuN, PuN_2.	8505	DFT
		AnO_2^{2+}; An=U,Pu. Their nitrates, sulfates.	7297	PP
		AnO_2^{2+}; An=U,Pu.	8136	PP
		$AnO_2^{2+}\cdot nH_2O$; An=U,Pu; n=0,4-6.	9808	PP
		n=5 most stable.		
		PuO_2^{2+} excited states.	8815	PP
		$Pu(H_2O)_n^{3+}$ clusters, n=6...12.	6966	PP
		n = 8 or 9 preferred.		
		$An(C_8H_8)_2$; An=U-Pu.	7151	PP
		$An(C_6H_3R_3)_2$; An=Th,U,Pu; R=Me,^{t}Bu.	8620	DFT
		$(AnO_2)(NO_3)_2\cdot 2$(TEP); An=U,Np,Pu; TEP=triethyl phosphate.	8026	DFT-DVM
95	Am	AnO_2^{2+}, $HOAnO^{2+}$, $An(OH)_2^{2+}$; An=U-Am.	10065	PP

Element		Compounds	Ref.	Method
		$An(Ch)_2$; An=Th-Am; Ch=η^7-C_7H_7. Also UCh_2^-.	8619	DFT
		$An(Bz)_2$; An=Th-Am; Bz=C_6H_6.	8620	DFT
103	Lr	AnH, AnF, AnO; An=Ac,Lr. Actinide contraction.	8485	PP
		MF, MH, MH_3; M=Ac,Lr. Lanthanide and actinide contractions.	8550	DF+MP2
104	Rf	$RfCl_4$. R/NR.	8788	DFB
105	Db	MO; M=Nb,Ta,E105	7484	PP
		MCl_5; M=Nb,Ta,Db. Bonding trends.	9198	DV DVM
		MCl_4; M=Zr-Rf, MCl_5; M=Nb-Db, MCl_6; M=Mo-Sg.	9199	DV DFT
		MOX_3; M=V-Ta,Pa,Db; X=Cl,Br.	8114,8122	DFT
		MX_6^-; M=Nb,Ta,Pa,Db; X=F,Br.	9196	DV DFT
		$M(OH_2)_6^{5+}$; M=Nb,Ta,Pa,Db.	9194	DV DFT
		$M(OH)_nCl_{6-n}^-$, $MOCl_4^-$, $MOCl_5^{2-}$; M=Nb,Ta,Pa,Db.	9195	DV DFT
106	Sg	Halides of Groups 4-6.	8118,8122	DFT
		$M(CO)_6$; M=Cr-W,U,Sg.	9030,9035	PP
		$[MO_4]^{2-}$; M=Cr-Sg.	9200	DV DFT
		$MOCl_4$; M=Mo-Sg.	9201	DV DFT
		MO_2Cl_2; M=Cr-Sg.	9202	DV DFT
111		MH; M=Cu-E111.	9684	PP
		MF_n^-; M=Cu-E111; n=2,4,6.	9677	PP
		MX; X=H,F-Br,O,Au. M_2; M=Au,E111. SO effects.	8695	DFT
112		$(E112)H^+$, $(E112)F_2$, $(E112)F_4$.	9683	PP
113		(113)H, (113)F.	7955	PP
		$(113)X_n$; n=1,3,5; X=H,F-I.	9685	PP
114		MH; M=Sn-E114.	9031	PP
		MX_2, MX_4, M=C-E114, X=H,F,Cl.	9679	PP
117		(117)H.	7955	PP
		XH; X=I,At,E117.	9572	DF
		XH; X=Br-E117. $7p8s$ hybridization!	9034	PP
118		RgF_n; n=2,4; Rg=Xe,Rn,E118.	7958	PP
		RgF_4; Rg=Xe-E118.	9031,9032	PP

Chapter 8

Solid-State Theory

Table 8.1: Band-structure calculations.

Reference	Comments
Bucher (1990)	Cohesive properties of AgCl. Van der Waals important.
Z. W. Lu et al. (1991b)	Long-range order in PtX; X=Ni,Cu,Rh,Pd. In PtNi, Pt 6*s* stabilization promotes ordering, not phase separation.
Troullier and Martins (1991)	PP for plane-wave calculations. R/NR Cu.
Cooper et al. (1992)	Surface electronic structure and chemisorption. U, Pu.
Richter et al. (1992,1995)	Crystal-field parameters of $SmCo_5$ obtained from a solid-state ab initio calculation.
Saalfrank (1992)	Quantum size effects in thin lead films. Pb(111).
Shik et al. (1992)	Methods for electronic structure and magnetic properties of substitutional impurities in regular crystals.
Solov'ev (1992)	AnC, AnN; An=U→Pu. Electron structure and magnetic properties.
Ahuja et al. (1993)	High-pressure phases of Ti, Zr, Hf.
Aldén et al. (1993)	Core-level shifts at surface for 4*d* and 5*d* metals.
Antonov et al. (1993a)	Optical properties of cubic 5*d* metals.
Antonov et al. (1993b)	Optical properties of hcp 5*d* metals.
Antonov et al. (1993a)	Optical properties of actinides.
Bauer et al. (1993)	$GdAl_2$. ^{27}Al Knight shift, ^{157}Gd E2 hfs.
Bose et al. (1993)	Semiconducting $CsSnBr_3$.
Braun and Borstel (1993)	Photoemission from GaAs(110).
de Mello et al. (1993)	Zr, Hf. Electric field gradient.
Eibler et al. (1993)	Unreconstructed Au(001) surface.
B.-S. Fang et al. (1993)	SO effects on electronic structures of Nb(001).
Fernández Guillermet et al. (1993)	Cohesive properties of 5*d*-metal carbides and nitrides with NaCl structure.
Fiorentini et al. (1993)	Reconstruction mechanism of fcc TM (001) surfaces. Close-packed quasihexagonal reconstruction occurs for 5*d* metals Ir,Pt,Au, but does not occur for the 4*d* metals Rh,Pd,Ag. Driven by relativistically induced 5*d* charge depletion on surface.
Hao et al. (1993)	Surface electronic structure of γ-U.
Hemstreet et al. (1993)	SO PP for solids. III-V semiconductors.
Hjelm and Calais (1993)	SCF calculations of Zeeman splittings in metals.
Hjelm et al. (1993)	Induced magnetism in U metal. *L* and *S* parallel, opposite to Hund's third rule.
Jäger et al. (1993)	Ca_3AuN is an $Au^-N^{3-}\cdot 2e^-$ auride subnitride. Compared with Al_2Au, CsAu.
Jepson and Anderson (1993)	Electronic structure of hcp Yb.
Johansson and Brooks (1993)	Theory of cohesion in lanthanides and actinides.
Koshibae et al. (1993)	Cuprates with SO interaction.
Lovatt et al. (1993)	Relativistic spin-polarized scattering theory for space-filling potentials.
Massidda et al. (1993)	HF-LAPW approach.
Mendez et al. (1993)	Transfer matrix method for 1D band structures.
Moruzzi and Marcus (1993)	Trends in bulk moduli of 3*d* and 4*d* metals. Relativistic corrections counterproductive.
Ozoliņš and Körling (1993)	Structural properties of 3*d*, 4*d*, 5*d* TM. GGA.
Papanikolau et al. (1993)	Also 5*d* and some *sp* impurities (B,C,N) in alkali

Reference	Comments
	metals can be magnetic.
Pick and Mikušik (1993)	Pd and Pt overlayers on W(011).
Postnikov et al. (1993)	Ferroelectric structure of $KNbO_3$ and $KTaO_3$.
Romanov (1993)	Origin of linear terms in quasi-2D dispersion law. SO.
Safonov (1993)	Crystal-field anisotropies handled via the metric tensor of the space-time, for Dirac electrons.
Shick and Gubanov (1993)	An impurities in Th; An=U,Np,Pu.
Smelyansky et al. (1993)	Conduction-electron g-factors in noble metals.
Stahler et al. (1993)	Magnetic K-edge absorption in $3d$ elements. Relation to magnetic structure.
Thole et al. (1993)	Multiplet FS in photoemission of Gd and Tb $5p$ levels.
Timms and Cooper (1993)	Electron momentum distribution in Pb.
Weinberger et al. (1993ab)	Effective pair interactions in the Au-Pd system.
J. H. Xu et al. (1993)	Tight-binding theory of rhombohedral As,Sb,Bi including SO.
L. H. Yang et al. (1993)	Effect of $(n-1)p$ semicore banding on lattice constants of K-Cs. Increase by 2-3 %. Comes from hybridization with valence orbitals, not from direct overlap.
Agassi and Restorff (1994)	Inclusion of SO in band-structure calculations along a symmetry axis. PP. Cylindrical coordinate multipoles. PbSe[111].
Ahuja et al. (1994a)	Magnetism of Gd and Tb.
Ahuja et al. (1994b)	Optical properties of PdO and PtO.
Ahuja et al. (1994c)	Fermi surface of noble metals (Cu,Ag,Au).
Ahuja et al. (1994d)	Influence of semicore states on high-pressure phases of transition metals (Y, ... Pt).
Basu et al. (1994)	Localization of rel. electrons in a 1D disordered system.
Drchal et al. (1994)	Random alloys and their surfaces. Tested on fcc $Cu_{75}Au_{25}$.
Faulkner (1994)	Scattering matrices for non-spherical SR potential.
Jeon et al. (1994)	X-ray absorption studies of d occupancies of $4d/5d$ transition metals, compounded with Group III/IV ligands.
Kalpana et al. (1994)	Phase stability of BaE; E=S-Te.
Kaupp and von Schnering (1994c)	Crystal HF for MF_2; M=Cd, Hg. R/NR for Hg.
Kirchhoff et al. (1994a)	Solid Te. Polymorphs under pressure.
Kirchhoff et al. (1994b)	Solid AgCl.
Kirchner (1994)	DFT studies of adsorption to metal surfaces. Thesis. Ar/Ag(111), Ag/Si(111), O/Ge(001), Sb/Ge.
Markendorf et al. (1994)	Hcp TM ($3d-5d$, Sc,...,Os). NMR spin-lattice relaxation.
Munzar and Christensen (1994)	Sn/Ge superlattices.
K.-T. Park et al. (1994)	MO; M=Pd,Pt,Ag.
Reinisch and Bross (1994)	Total energy and Fermi surface of gold.
Shick and Gubanov (1994)	An impurities in bcc Fe; An=U,Np,Pu.
Singh (1994ab)	Relativistic effects in Zn, Cd and Hg. Mercury crystal structure due to relativity.
Söderlind et al. (1994,1995)	Ce, Th→Pu. Electronic properties using GGA.
Steinbeck et al. (1994)	Obtain crystal-field parameters for the $4f$ states of Er and Dy in Ag or Au from solid-state DFT calculations.
Svane (1994,1996)	Ce. α phase has delocalized $4f$ electrons.
Weinberger et al. (1994)	Cu-Au alloys.

Reference	Comments
Würde et al. (1994)	Surface electronic structure of Pb(001), (110), (111). $6s, 6p$ bands decoupled.
Antonov et al. (1995)	Magneto-optical properties of ferromagnetic metals.
Boisvert et al. (1995)	Diffusion on (100), (111) surfaces of Ag, Au, Ir. Ag, Ir (111) barriers equal melting point, Au one is twice it.
Brooks et al. (1995)	Review on trends from TM to Ln and An.
Burdett and Sevov (1995)	Stability of oxidation states of Cu. Oxides. SR LMTO. Also Ag, Au.
Bzowski et al. (1995a)	Ag or Au overlayers on Ru(001).
Bzowski et al. (1995b)	Au-M intermetallics; M=Al-In, Sn→Te.
Costa Cabral and Silva Fernandes (1995)	Dynamics and structure of molten CsAu. Au^- dimers at $R \sim 3$ Å found.
Dronskowski (1995)	In_2ThBr_6. $6d$ bonding for Th.
Dufek et al. (1995)	Iron compounds. Yield a new $^{57}Fe^*$ nuclear quadrupole moment.
Fast et al. (1995)	Elastic constants of hexagonal transition metals.
Grin et al. (1995)	Hyperbolic lone pair structure in $RhBi_4$.
Hammer and Nørskov (1995)	H_2 on M(111); M=Ni,Cu,Pt,Au. 'Why gold is the noblest of all metals.' Relativity not mentioned.
M. Heinemann et al. (1995)	β-PbO_2. Semimetal.
Hota et al. (1995)	PbTe. ^{207}Pb NMR shifts including SO effects.
Johansson et al. (1995)	Fcc Th. Stabilized by $5f$.
Krasovska et al. (1995)	RuO_2. Optical and photoelectron spectra.
Kwon et al. (1995)	Solid Ar and Kr under high pressure. $V/V_0 = 1$ to 0.1.
Y. Liu and Allen (1995)	Sb, Bi. TB+SO.
Medvedeva et al. (1995,1996)	δ-Bi_2O_3 with or without oxygen defects.
Z. W. Lu et al. (1995)	M_3X; M=Pd,Pt; X=Sc-Cu. Spin-polarization-induced structural selectivity.
Miyazaki et al. (1995)	DCNQI-(Cu,Ag) systems.
Paulus et al. (1995)	Group-4 semiconductors (C-Sn, diamond structure). HF + correlation from clusters. PP.
Sandratskii and Kübler (1995,1999)	Magnetic structures of uranium compounds. Effects of relativity (SO) and symmetry.
Terpstra et al. (1995)	PbO. red and yellow. Pb $6s^2$ hybridizes with O $2p$ and does not form an 'inert pair'.
Willatzen et al. (1995)	II-VI zinc blende materials. SO parameters and electron g-factor.
C. J. Wu et al. (1995)	Ta (100) and (110) surfaces.
R.-Q. Wu (1995)	Bimetallic interface Pd/Ta(110).
Ahuja et al. (1996)	Electronic and optical properties of HgI_2.
Becker et al. (1996)	Pu_3X; X=Al-Tl. Covalency between Pu df and X p.
Bei der Kellen and Freeman (1996)	Self-consistent relativistic full-potential Korringa-Kohn-Rostoker total-energy method. Pd, Ir, Pt, Au. InSb etc.
Charpentier et al. (1996)	Ba, α-Ce, Th.
X.-J. Chen et al. (1996)	II-VI semiconductors, Zn-Hg, S-Po. Cation-d–anion-p hybridization.
Cortona and Villafiorita Monteleone (1996)	Cohesion and structure of MO; M=Mg-Ba.
Delin et al. (1996)	Optical properties of MC, MN, MO; M=Ti-Hf.
de Wijs et al. (1996)	First-principles MD of liquid Mg_3Bi_2.

Reference	Comments
C. M. Fang et al. (1996)	$Pb_{1/3}TaS_2$.
Gasche et al. (1996)	Optical properties of Th, Pa, U.
Grosch and Range (1996)	MAu; M=Li-Cs. LiAu metallic, others ionic. The NaCl, CsCl and NaTl structures compared.
Grosch and Range (1996b)	MAu_5; M=Na-Cs.
Hjelm et al. (1996)	WO_3, MWO_3; M=Li,Na,H, H_2WO_3. Optical properties. H forms a hydroxide, alkalis give electrons to $5d$ band.
Karzel et al. (1996)	ZnO, ZnSe. Mössbauer isomer shift, (wurzite) EFG.
Mehl (1996)	Structure of Hg.
Mejías (1996)	Adsorption of Cu-Au on NaCl(001) surface. Cluster models.
Mian et al. (1996)	Solid galena, PbS. HF. Different PP, correlation corrections compared.
F. Nogueira et al. (1996)	Transferability of *local* PP, based on solid-state electron density. Good for Na, useful for K-Cs, Mg, Al-Tl, Sn-Pb, poor for Li, Be, Ca-Ba.
Paulus et al. (1996)	Cohesive energies for III-V semiconductors (BN to InSb, with ZnS structure). Localized-orbital CCSD. PP.
Pick (1997)	CO chemisorption on Pt(111).
Richter et al. (1996)	U_2Pd_2M; M=In,Sn. Giant magnetoresistance.
Shick et al. (1996)	Relativistic Green's function method for electric and magnetic properties of random alloys. Ferromagnetic $3d$ metals. Fcc alloys $Co_{50}M_{50}$; M=Ni,Pt.
Springborg and Albers (1996)	Electronic structure of Pt in polyyne, $[Pt(PH_3)_2C_6]_x$.
Steinbeck et al. (1996)	Obtain crystal-field parameters for the $4f$ states of Sm in Fe and Co intermetallics from solid-state DFT calculations.
Weinberger et al. (1996)	'Band structure' and electrical conductivity of disordered layered systems.
Akella et al. (1997)	High-pressure phases of U.
Amirthakumari et al. (1997)	High-pressure phases of alkali halides.
Asokamani et al. (1997)	$AgGaX_2$, X=S-Te.
Brooks et al. (1997)	Crystal field excitations of Ln are combined from $4f$ excitations and a cloud of shielding conduction electrons. Spin Hamiltonians of TmSb and PrSb as examples.
Celestini et al. (1997)	'Hexatic' order on surface of liquid Au? Here MD simulation. Relativistic $5d-6s$ shifts shorten surface bonds of Ir, Pt, Au. See Fiorentini et al. (1993).
Ebert et al. (1997c)	Relativistic band structure of disordered magnetic alloys.
C. M. Fang et al. (1997)	ReS_2, $ReSe_2$, TcS_2.
Fehrenbach and Schmidt (1997)	Test the relativistic kinetic energy operator in spline-augmented plane-wave calculations.
Fleszar et al. (1997)	One-electron excitations and the plasmon in Cs metal. $5p$ semicore correlation shifts plasmon energy. 'Why is Cs yellow?'
Geipel and Hess (1997)	DK approach for solids (in crystal HF). Ag, AgX; X=F-Br. Bond contraction. Metal stabilized, salts destabilized by relativity.
Hwang et al. (1997)	Pr.
Karki et al. (1997)	$AgGaSe_2$. Elasticity and lattice dynamics.
Knöpfle et al. (1997)	U_3Sb_4. Symmetry properties of intra-atomic spin

Reference	Comments
	and angular-momentum densities.
Kollár et al. (1997)	α-Pu. GGA works.
Ladik (1997)	DF equations for solids.
M.-S. Liao et al. (1997)	CH_4+M(111); M=Ni-Pt,Cu.
M.-S. Liao and Schwarz (1997b;1999)	Hg_2L_2; L=F-I. Molecules and solids.
Lorenzana et al. (1997)	PbF_2: high-pressure phases.
Mishra et al. (1997)	Bi_2Se_3, Bi_2Te_3 including SO. Electronic structure and thermoelectric properties.
Pénicaud (1997)	δ-Pu, Es. Electron localization.
C. Persson and Lindefelt (1997)	SiC polytypes. SO important on hole masses.
Philipsen et al. (1997)	CO adsorption on (111) surfaces of Ni,Pd,Pt.
Ravindran et al. (1997)	Optical properties of monoclinic SnI_2.
Raybaud et al. (1997ab)	TM sulfides. Crystal and electronic structure. Catalytic activity related to TM-S bond energy.
Schmidt and Springborg (1997)	Linear or zig-zag chains of Tl,Pb,Bi.
Sekine et al. (1997)	TiC and UC: a comparison.
Severin et al. (1997)	Core M1 hfs of ferromagnetic Fe, Co, Ni.
Söderlind and Eriksson (1997)	Pa. Pressure-induced phase transitions.
Söderlind et al. (1997)	Structures of Pu.
Solanki et al. (1997)	Optical properties of HgI_2
Stachiotti et al. (1997)	ReO_3 and related oxides.
Svane et al. (1997)	Hfs parameters in tin compounds.
Terpstra et al. (1997)	Pb_3O_4, a mixed-valence compound.
Victora (1997)	AgX; X=Cl-I. Band structure.
Vitos et al. (1997)	Atomic volume of α-phase Fr$\rightarrow$Pu. Itinerant $5f$ found in Th to Pu.
Wei and Zunger (1997)	PbE; E=S-Te. The Pb $6s$ band below Fermi level leads to band structure anomalies.
Younk and Kunz (1997)	Solid $Pb(N_3)_2$. Band structure supports Gilman detonation model.
Zeng et al. (1997)	Ba under high pressure. Hexagonal close-packed phase. Transfer from $6s$ to $5d$ crucial in the decrease of c/a ratio.
Ahuja et al. (1998a)	High-pressure phases of CsH.
Ahuja et al. (1998b)	High-pressure phases of Sr.
Boettger (1998)	SR LCGTO. Applied on Au.
Boettger (1998b, 1999)	Phases of Mo. R/NR.
Boucher and Rousseau (1998)	Cs_3Te_{22}. Te-Te contacts ca. 340 pm. Two $CsTe_6$ slabs + four Cs Te_3 layers in unit cell.
Boykin (1998)	SO effects in tight-binding models. GaSb.
Deb and Chatterjee (1998)	Electronic structure and bonding of Ag_2O.
Delin et al. (1998ab)	Cohesive properties of lanthanides. Effect of generalized gradient corrections.
Delin et al. (1998c)	PbCh; Ch=S-Te.
S.-Q. Deng et al. (1998)	EHT band structure of Hg. Superconductivity discussed.
Doublet et al. (1998)	Electrical properties of TiX_2; X=S-Te. QR/NR.
Dudešek et al. (1998)	GaN. Ga-$3d$-to-N-$2s$ bonding.
Hu et al. (1998)	Band-structure version of the DF code MOLFDIR. Application to a $1D$ chain of Se.

Reference	Comments
Huhne et al. (1998)	Relativistic KKR method. Bcc Fe, fcc Co, fcc Ni.
Kokko and Das (1998)	Ground-state properties of $3d$ and $4d$ metals. GGA.
Krasovska et al. (1998)	The colour of sulphur. Electronic.
M.-S. Liao et al. (1998)	CN^- adsorption on M(100) electrodes; M=Cu-Au.
M.-S. Liao and Zhang (1998b)	CH_4 dissociation on Ru,Rh-Ir,Ni-Pt,Cu-Au.
Löken et al. (1998)	$Tl_2Au_4S_3$. Au-Au and Au-S interactions.
Lundin et al. (1998)	Hard MO_2; M=Ru,Os. Latter harder.
Maehira et al. (1998)	UC Fermi surface.
Miyagi et al. (1998)	Br_2, I_2 under high pressure.
Nemoshkalenko and Antonov (1998)	Computational methods in solid-state physics. Book.
Nunes et al. (1998ab)	Solid AgX; X=Cl-I. Pressure-induced phase transitions.
Ozoliņš et al. (1998)	Cu-Ag, Ag-Au, Cu-Ag and Ni-Au intermetallics. Phase diagrams and structures.
Papakondylis and Sautet (1996)	α-MoO_3. Crystal HF. H_2O, CO adsorption.
Patnaik et al. (1998)	PbTe. Nuclear spin-spin coupling.
Pavone et al. (1998)	Sn. $\alpha \leftrightarrow \beta$ phase transition. Entropy driven, due to different vibrational spectra.
Ravindran et al. (1998)	High-pressure phases of Ce.
Sághi-Szabó et al. (1998)	Piezoelectricity in $PbTiO_3$.
Seifert et al. (1998)	DFT with Car-Parrinello for Zintl systems. Liquid NaSn.
Seshadri et al. (1998)	Metal-metal bonding and metallic behaviour of some ABO_2 Delafossites. $AgMO_2$; M=Fe,Co,Ni. $MCoO_2$; M=Pd,Pt.
Sigalas et al. (1998)	Average interstitial electron densities for alkali, noble and transition metals. Related to cohesive energy.
Söderlind (1998)	Theory of the crystal structures of Ce, early An. Review.
Söderlind and Moriarty (1998)	Ta up to 10 Mbar.
Strange (1998)	Relativistic QM with condensed-matter and atomic physics applications. Book.
Vogel et al. (1998)	Solid AgX; X=Cl-I.
Yamagami (1998)	All-electron spin-polarized relativistic LAPW method. Bcc Fe, hcp Gd, U monochacogenides.
Yamaguchi and Miyagi (1998)	Molecular solid I_2 under pressure. SR. Transition from molecular phase to monatomic body-centred orthorombic (bco) phase.
Yoo et al. (1998)	Phase diagram of U at high p and T.
Y. Zhang et al. (1998)	Scheelite materials AMO_4; A=Ca,Pb; M=Mo,W.
Alatalo et al. (1999)	Truncated pseudopotentials for alloy calculations. Cut-offs in momentum space introduced. Pd, Pd-Al alloys as example.
Asato et al. (1999)	Full-potential KKR calculations for metals and semi-conductors. Lattice parameters, bulk moduli agree with other FP methods. Fe,Ni,Cu; Rh,Pd,Ag.
Boettger et al. (1999)	Phases of U.
Bose (1999)	Electronic structure of liquid mercury.
Carlesi et al. (1999)	Cs under pressure.
de Wijs and de Groot (1999)	Amorphous WO_3. W-W bonds of <3 Å occur.
Fehrenbach (1999); Fehrenbach and Bross (1999)	SR spline augmented plane-wave method. DK. Ag, Au. Pd. GaN.

Reference	Comments
Filonov et al. (1999)	Isostructural Ru and Os silicides and germanides. Os has larger gaps than Ru.
Ge and King (1999)	CO chemisorption on Pt(110). Slab model.
Hemmingsen et al. (1999)	Structure and EFG:s in β-$Cd(OH)_2$.
Korzhavyi et al. (1999)	Vacancy formation energy in transition and noble metals.
Krasovskii (1999)	Fe-Ni compounds at the Earth's core conditions.
Lalić et al. (1999)	Hf_2Fe. EFG.
Landrum et al. (1999)	Ce(III) versus Ce(IV) nitrides and other solids. Odd electron in CeN more d than f.
Liubich et al. (1999)	Interstitial B in W.
Lowther et al. (1999)	Relative stability of ZrO_2 and HfO_2 structural phases.
Miyazaki and Ohno (1999)	Solid $(Me_4N)[M(dmit)_2]_2$; M=Ni,Pd.
Okamoto and Takayanagi (1999)	Infinite 1D chain of gold atoms. Structure and conductance.
Pacchioni et al. (1999)	TM core level shifts upon adsorption on Al_{37} model of Al(100). 'TM'=Ne,K,Cu-Au,Ni-Pt. Covalent interaction.
Rościszewski et al. (1999)	Cohesion of rare-gas crystals, Ne-Xe. Three-body contributions nearly 7% for Xe.
Rotenberg et al. (1999)	SO-induced surface band splitting in Li/M(110); M=Mo,W. A probe on surface potential gradient. Experimental.
Schmid et al. (1999)	Relativistic GGA tested on 5d TM. Band structure and cohesive properties. Pt, Au.
Senda et al. (1999)	Liquid K-Pb alloys. Pb_4^{4-} Zintl ions found.
Shick et al. (1999)	Electronic structure and phase transitions of Bi.
Shishidou et al. (1999)	5f orbital magnetic moment of US.
Sökeland et al. (1999)	Separability of relativistic electron propagators. Scattering matrices from Dirac-Green functions. Photoemission, PES.
Solimar and Abelraheem (1999)	Modification of band structure in intense laser fields. 1D model. New gaps introduced.
Springborg (1999)	PtS_2 chains. 3D K_2PtS_2.
Suzuki and Nakao (1999)	Fully relativistic LCAO approach for crystals. Au, InSb. R/NR.
Temmerman et al. (1999)	Electronic configuration of Yb compounds. Yb(II) versus Yb(III).
Tse et al. (1999)	K-Ag intermetallics at high pressure. Claims Ag-Ag bonding interactions at 554 pm, finds short K-K distances of 339 pm. Ag^+ form hexagonal layers, interlayer Ag-Ag 360 pm.
Voss et al. (1999)	WSe_2.
Watson et al. (1999)	Ab initio calculation reproduces the distorted structure of solid α-PbO. The 'sterically active lone pair' has, however, Pb 6s - O 2p hybridization. Cp. Terpstra et al. (1995).
Xie et al. (1999)	Ag. Thermal properties in quasiharmonic approximation.

Table 8.2: Relativistic theories of solid- and liquid-state phenomena.

Reference	Comments
Abrikosov and Gor'kov (1962)	SO interactions and the Knight shift in superconductors.
Appel (1965)	SO effect on Knight shift of main-group superconductors.
Ham (1965)	Quenching of SO by dynamical Jahn-Teller effects.
Akai et al. (1990)	Theory of hyperfine interactions in metals.
Alouani and Albers (1993)	Magnetism in linear MX chains, M=Ni,Pt, X=Cl-I.
Balcar and Lovesey (1993)	Magnetic neutron spectroscopic intensities of Sm.

Reference	Comments
Bonesteel (1993)	SO scattering and pair breaking in disordered Cu-O layer.
Chalker et al. (1993)	Correlations at mobility edge in a 2D system with SO scattering. Anderson metal-insulator transition.
Coehoorn and Buschow (1993)	Hfs field at Gd nuclei in intermetallic compounds.
Eberhart et al. (1993)	Mechanisms of fracture. Why is CuAu ductile but TiAl brittle. Transition state for decohesion sought.
Ebert and Akai (1993)	Relativistic effects on hfs of TM.
Ebert et al. (1993)	Magnetic x-ray dichroism in dilute and concentrated TM alloys.
Godfree and Staunton (1993)	Relativistic approach to magnetic anisotropy.
Halilov et al. (1993)	Photoemission from magnetic compounds.
J. Luo et al. (1993)	Scattering operator for elastic and inelastic resonant x-ray scattering. Applied on Ln, An, TM.
Ramazashvili (1993)	Electron states in planar 2D ferromagnet. SO effects.
Reinisch and Bross (1993)	Relativistic effects on the Compton profile of polycrystalline gold.
Roy and Basu (1993ab)	Relativistic electrical conduction in disordered systems.
Schmiedeskamp et al. (1993)	Spin polarization in $5d$ photoemission from a Tl film.
Taylor and Gyorffy (1993)	Ferromagnetic monolayer with model SO and dipole-dipole interactions.
X. D. Wang et al. (1993)	Circular magnetic x-ray dichroism in heavy rare-earth metals.
Ebert and Guo (1994)	MXD spectra using spin-polarized relativistic LMTO.
Gotsis and Strange (1994)	Relativistic theory of x-ray Faraday effects.
Grass et al. (1994ab)	Theory of photoemission from solids.
Jenkins and Strange (1994)	Relativistic, spin-polarized single-site scattering theory.
Kulakowski et al. (1994)	Magnetic anisotropy and magnetostriction of atom pairs. SO.
Macêdo (1994)	Influence of SO scattering on electron-wave propagation in a disordered, quasi-1D medium.
Meir and Wingreen (1994)	SO scattering and the Kondo effect.
Meservey and Tedrow (1994)	Spin-polarized electron tunneling.
Ostanin and Shirokovskii (1994)	New method for magnetocrystalline anisotropy energy in relativistic ferromagnets.
Rajagopal (1994)	DFT including EM fields in condensed matter.
Tamura et al. (1994)	Linear and circular dichroism in angle-resolved Fe $3p$ photoemission.
Tyson (1994)	Relativistic effects in x-ray-absorption fine structure.
Yildirim et al. (1994)	Symmetry, SO and spin anisotropies: A spin anisotropy can only arise for tetragonal symmetry, if both SO and Coulomb exchange is included. Magnetic insulators.
Campbell and Segre (1995)	SO-induced lattice instabilities for half-filled hopping Hamiltonian.
Capelle et al. (1995)	Relativistic theory of superconductivity.
Cole et al. (1995)	Auger parameter shifts from free atoms to solids, in alkali and alkaline earth metals.
Evangelou (1995)	Anderson transition in presence of SO coupling. 2D disordered systems considered.
Fluchtmann et al. (1995)	R full-potential photoemission theory for ferromagnetic materials.
Fuks et al. (1995)	Solid and liquid W using effective potential.

Reference	Comments
Jenkins and Strange (1995)	X-ray magnetic dichroism in random substitutional alloys of f-electron elements.
Kraft et al. (1995)	Magneto-optical Kerr spectra on UX surfaces, X=S-Te.
Tamura et al. (1995)	X-ray absorption near edge structure in metals. Relativistic effects and core-hole screening.
Újfalussy et al. (1995)	Magnetism of $4d$ and $5d$ adlayers on Ag(001) and Au(001). R/NR. Relativity kills magnetism for Ir mono- and Pt double layers.
Wolff et al. (1995)	Self-consistent SO and Zeeman terms in otherwise NR ab initio calculations. Magnetic structure factors for $CsCoCl_5$.
Zakharov and Cohen (1995)	Structural, electronic, vibrational and super-conducting properties of sulfur under high pressure.
Adrian (1996)	Conduction-electron spin relaxation in M_3C_{60}, M=K,Rb,
Continenza et al. (1996)	Optical conductivity of $YbCu_4AM$; M=Ag,Au.
Ebert (1996)	Review on magneto-optical effects in TM systems.
Ebert et al. (1996); Ebert et al. (1997b)	SO effects for Dirac equation and spin-dependent potentials divided into two parts, diagonal and off-diagonal. Applications to magneto-optical Kerr effect, SO-induced orbital moments.
Ebert and Schütz (1996)	SO-influenced spectroscopies of magnetic solids. Book.
Kuch et al. (1996)	Magnetic dichroism of perpendicularly magnetized Ni/Cu(001)
Rajagopal and Buot (1996)	Fundamentals of time-dependent DFT, including EM fields.
Roy (1996)	'Fibonacci lattice' of rectangular potential wells. Landauer resistance.
Vargas et al. (1996)	Electronic energy loss of low-energy protons, channeled in single-crystal Au ⟨100⟩ direction.
Ankudinov and Rehr (1997)	Relativistic theory of XAS and XMCD.
Arola et al. (1997)	Magnetic x-ray scattering from ferromagnetic Fe.
Capelle et al. (1997,1998)	Theory of dichroism for superconductors.
Ebert et al. (1997a)	Current density functional theory and spontaneous magnetization of solids. Large SO effects in Fe, Co. (Vignale-Rasolt theory.)
Grimaldi and Fulde (1997)	Screening of phonon-modulated SO interaction in metals. Comes from the spin-other-orbit term.
Kresse and Hafner (1997)	Metal/nonmetal transition in expanded fluid Hg. Occurs at 8.8 g cm^{-1}.
Moreau et al. (1997)	Relativistic effects in electron-energy-loss-spectroscopy on the Si/SiO_2 interface plasmon peak.
Oja and Lounasmaa (1997)	Nuclear magnetic ordering of simple metals.
Pollack et al. (1997)	Test of density-based local pseudopotential on 16 simple metals. Phonon spectra, bulk and shear moduli, resistivities.
Qian et al. (1997)	Persistent currents from competition between Zeeman coupling and SO interaction.
Arola and Strange (1998)	Magnetic x-ray scattering from single Cu crystals.
Delin et al. (1998ab)	Effect of GGA on lanthanide cohesive properties.
Chamarro et al. (1998)	SO effects in semiconductor nanocrystals. (CdS, ca. 2 nm).
Doll and Stoll (1998)	Ground-state properties of heavy alkali halides.
Doll et al. (1998)	Closed-shell interaction in solid AgCl and AuCl.

Reference	Comments
Jenkins and Strange (1998)	Magnetic x-ray circular dichroism in TM alloys.
E. Kim and Cox (1998)	Knight-shift anomalies in heavy-electron materials.
Kiselev et al. (1998)	Electron g factor in 1D and 0D semiconductor nanostructures (quantum wires and quantum dots).
Lyanda-Geller (1998)	Quantum interference and electron-electron interactions at strong SO coupling in disordered systems.
Petrilli et al. (1998)	EFG calculations using the projector augmented wave method.
Rajagopal and Mochena (1998)	SO interaction in many-body theory of magnetic electron systems. Includes two-electron SO.
Újsághy et al. (1998)	SO-induced magnetic anisotropy for impurities in metals. Finite-size effects in Kondo resistivity.
Bulgakov et al. (1999)	SO-induced Hall-like effect.
Capelle and Gross (1999a)	Dirac equation for superconductors.
Capelle and Gross (1999b)	Pauli equation for superconductors.
G.-H. Chen and Raikh (1999)	Exchange-induced SO effects in 2D systems. Effects on g-factor.
Ebert et al. (1999a)	Fully relativistic description of static M1 hfs in magnetic and nonmagnetic solids.
Ebert et al. (1999b)	Fully relativistic theory of magnetic EXAFS. Nonspherical potentials allowed. Ni, Pt, Fe_3Pt.
Ebert et al. (1999d)	Influence of SO and a current-dependent potential on residual resistivity of disordered magnetic alloys.
Huhne and Ebert (1999)	Fully relativistic description of magneto-optical properties of arbitrary layered systems.
Moroz and Barnes (1999)	SO effect on band structure and conductance of quasi-one-dimensional systems.

Chapter 9

Relativistic Effects and Heavy-Element Chemistry

Table 9.1: "Relativity and the periodic system". Periodic trends, reviews and pedagogical papers.

Reference	Comments
Petrucci (1989); Petrucci and Harwood (1993)	General chemistry textbook. Quotes relativistic effects.
Z. W. Lu et al. (1991b)	Long-range order in PtX; X=Ni,Cu,Rh,Pd. In PtNi, Pt 6*s* stabilization promotes ordering, not phase separation.
Haire and Gibson (1992)	Position of Pu among actinide metals and compounds.
D. C. Hoffman (1992)	Nuclear and chemical properties of E103-E105.
Sharpe (1992)	Inorganic chemistry textbook. Quotes relativity.
Yarkony (1992)	Spin-forbidden chemistry within BP approximation. Review.
Huheey et al. (1993)	Inorganic chemistry textbook. Quotes relativity.
Johansson and Brooks (1993)	Theory of cohesion in lanthanides and actinides.
Kaupp and Schleyer (1993a)	Why inorganic Pb(II) but organic Pb(IV)? Bent's rule for bond angles holds.
Kaupp and von Schnering (1993)	Proposal for the Hg(IV) compound HgF_4.
Kudo et al. (1993)	Review on strained, polycyclic compounds with M_n skeletons (M=Si-Pb).
Lambert et al. (1993)	'Inverted electronegativity' of Li and Na.
L. Li et al. (1993)	Experimental reactions of M_2; M=Cu-Au with O_2, N_2O, N_2, H_2, CH_4, CO, CO_2, C_2H_4 in the gas phase. Au_2 anomalous. Reasons discussed.
Norman and Koelling (1993)	Electronic structure of *f* electron metals.
Pisani et al. (1993)	Discuss relativistic effects in atoms and molecules using LCAO calculations on H-like systems as example.
Schwerdtfeger et al. (1993)	The Hg-Hg bond in inorganic and organometallic chemistry.
Umland (1993); Umland and Bellama (1996)	General chemistry textbook. Quotes the Dirac equation.
Eliav et al. (1994e)	Ground state of E111 (eka-Au) d^9s^2, not $d^{10}s^1$.
D. C. Hoffman (1994,1996); D. C. Hoffman and Lee (1999)	The heaviest elements.
Kaupp and von Schnering (1994a)	Dimerization of HgX_2; X=F-I. R: Weak C_{2h} dimers. NR: Covalent D_{2h} structures.
Kaupp and von Schnering (1994b)	Stability of Hg_2^{2+} attributed to differential solvation/aggregation effects in the condensed phase. Gas-phase $Hg_2X_2 \leftrightarrow HgX_2$+Hg shifted to right!
Klapötke and Tornieporth-Oetting (1994)	Textbook on main-group chemistry. Includes relativity.
M.-S. Liao and Schwarz (1994); M.-S. Liao and Schwarz (1997a); M.-S. Liao (1993)	Effective radii of monovalent coinage metals. For CN=2, Au(I) ca. 10 pm smaller than Ag(I).
W.-J. Liu and Li (1994)	Review on relativistic quantum chemistry.
Malli (1994ab)	Relativistic and electron correlation effects in molecules and solids.
Marian (1994)	Relativistic calculations on TM compounds.
Norman (1994,1997)	Periodicity and the *p*-block elements. School textbook. Mentions relativity.
Onoe et al. (1994ab); Onoe (1997)	Analyses relativistic effects on DVM-DFT MO:s for Cu_2, AuH, Pb_2, XF_6;X=S-Po, Mo-W,Re→Pt, U,Np,Pu.
Pershina and Fricke (1994a)	Highest chlorides of Rf→Sg.

Reference	Comments
Pershina et al. (1994a)	Physicochemical properties of Rf→Sg (E104-E106).
Pershina et al. (1994b)	Thermodynamic functions of Db (E105), deduced from atomic MCDF calculations.
Pershina et al. (1994c)	Complexation of Nb-Db in aqueous HCl solutions.
Ron et al. (1994)	Relativistic, retardation and multipole effects in atomic photoionization cross sections. Z, n, and l dependence.
Schwerdtfeger et al. (1994c)	Predict the existence of AuF.
Watson and Weinert (1994)	Charge transfer in gold–alkali-metal systems. 50/50 systems. Short Au-Au leads to metallic character for AuLi-AuK. AuRb, AuCs are semiconductors.
Wezenbeek et al. (1995)	H-MCl_3 bonds; M=Hf,Th. Relativity explains nearly half of the Th-H bond strength of 3.60 eV.
Hammer and Nørskov (1995)	H_2 on M(111); M=Ni,Cu,Pt,Au. 'Why gold is the noblest of all metals.' Relativity not mentioned.
Heinemann (1995)	Gas-phase ion-molecule chemistry. Experiment versus theory. Thesis.
Hess et al. (1995)	Review on SO effects and methods.
Holleman et al. (1995)	Inorganic chemistry textbook.
Kratz (1995)	Chemistry of the heaviest elements.
J. Li et al. (1995a)	$MH_4(PH_3)_3$; M=Fe-Os. Non-classical hydrides of Os due to relativity (cp. Pyykkö (1988a)[5680] p. 585).
Moc and Morokuma (1995, 1997)	Periodic trends in Group 15 (P-Bi). MX_5, MX_6^-, ...
Münzenberg (1995,1999)	Discovery of the heaviest elements.
Schädel (1995)	Chemistry of transactinides.
Seth et al. (1995)	Trends of atomic orbital energies and radii for Groups 11 (Cu-E111) to 15 (As-E115). Relativistic and shell-structure effects.
S. G. Wang and Schwarz (1995a)	LnH, LnF, LnO; Ln=La,Gd,Yb,Lu. Lanthanide contractions (La-Lu) 19, 10 and 5 pm, for H, F and O, respectively.
Yatsimirskii (1995)	Review on relativistic effects in chemistry.
Zumdahl (1995,1998)	General chemistry textbook. Quotes relativity.
Almlöf and Gropen (1996)	Review on relativistic effects in chemistry.
Bigeleisen (1996)	Nuclear size and shape effects in chemical reactions. Uranium redox reactions as example.
Cundari et al. (1996)	Review on pseudopotential methods.
Dolg and Stoll (1996)	Review on lanthanide chemistry.
Eliav et al. (1996b)	E118 (eka-Rn) first rare gas with electron affinity. Qualitative explanation the 8s LUMO stabilization.
Eliav et al. (1996c)	Is E113 (eka-Tl) a 6d transition metal?
Ionova et al. (1996a)	MOX_3; M=V-Ta,Pa,Db(E105); X=Cl,Br. Bonding trends.
Ionova et al. (1996b)	Atomic properties of Rf-Sg (E104-E106).
Ionova et al. (1996c)	Halides of Groups 4-6.
Ionova et al. (1996d)	Oxohalides of Group 6.
Ionova et al. (1996e)	Fugacity of halides and oxohalides of transition metals and transactinides. *Special comment:* According to V. Pershina, the preceeding papers Ionova (1996a-e) are unauthorized duplicates from her earlier papers.

Reference	Comments
Ionova et al. (1996f)	Sublimation enthalpy of $5d$ metals.
Kaupp et al. (1996b)	The 6th-row systems PoF_6^{2-}, AtF_6^-, RnF_6 octahedral, due to relativity. Their 5th-row analogues fluctuate.
Klapötke and Schulz (1996)	Quantum chemistry in main-group chemistry. Includes relativity.
Mackay et al. (1996)	Inorganic chemistry textbook. Includes relativity.
Musaev and Morokuma (1996)	Potential-energy surfaces of TM-catalyzed chemical reactions.
Neogrády et al. (1996)	QR CCSD(T) polarizabilities for M,M^+; M=Cu-Au. Ag > Au but $Ag^+ < Au^+$.
Pershina (1996)	Electronic structure and properties of transactinides and their compounds.
Roos et al. (1996)	Review multiconfiguration PT for molecules. Relativistic effects on optical properties of MCl_2; M=Sc,Cr,Ni.
Rösch et al. (1996)	DK DFT molecular calculations.
W. H. E. Schwarz et al. (1996)	Interpretation of relativistic effects on chemical bonding.
Seaborg (1996)	Evolution of the modern periodic table. Future sketched to E168.
Siegbahn (1996)	Electronic structure calculations for molecules containing transition metals.
Türler (1996)	Gas-phase chemistry of transactinides. Rf(E104), Db(E105).
Umemoto and Saito (1996)	Electron configurations of superheavy elements, Z=121-131. g-electrons appear at Z=126.
van der Lugt (1996)	Polyanions, especially Zintl anions, in ionic alloys A review.
Balasubramanian (1997ab)	Relativistic effects in chemistry.
Greenwood and Earnshaw (1997)	Chemistry of the elements. Textbook.
S. A. Cotton (1997)	Chemistry of precious metals. Treatise.
Fricke et al. (1997)	Review on superheavy elements. DVM.
Hess (1997)	Review on relativistic effects in heavy-element chemistry.
Janiak (1997)	Review on organothallium (I,II) chemistry.
Kaltsoyannis (1997a)	Review on relativistic effects in inorganic and organometallic chemistry.
Kaltsoyannis and Bursten (1997)	$Th(Cp)_3$. R $6d^1$, NR $5f^1$ ground state.
Küchle et al. (1997)	Lanthanide and actinide contractions. Depend on the ligand.
M.-S. Liao and Zhang (1997)	MH_x^{2-}, MCl_y^{2-}; M=Ni-Pt; x=2,4,6; y=4,6 in crystal field. Relativistic effects favour higher oxidation state.
Pacchioni et al. (1997)	CO adsorption on M; M=Ni-Pt. Relativistic trends.
Philipsen et al. (1997)	CO adsorption on (111) surfaces of Ni,Pd,Pt. Relativistic correction to CO/Pt adsorption energy 70% at SR level, 55% with SO included.
Pyykkö (1997)	Strong closed-shell interactions in inorganic chemistry. Review.
Schädel et al. (1997ab)	Experimental chemistry of Sg (E106).
Bartlett (1998)	Relativistic effects and the chemistry of gold.
Delley (1998)	Scattering-theory approach to scalar relativistic corrections to bonding. Local pseudopotential can include them.

Reference	Comments
Dolg (1998)	Lanthanides and actinides.
Günther et al. (1998)	Chromatographic extraction trend Zr>Rf>Hf in HCl/tributylphosphate.
Hess (1998)	Review on relativistic theory and applications in chemistry.
S. Hofmann (1998)	New elements – approaching Z=114.
Laerdahl et al. (1998)	MF, MH, MH_3; M=La,Lu,Ac,Lr. Lanthanide and actinide contractions. Relativity 10-30% of former, 40-50% of latter.
Mingos (1998)	'Essential trends in inorganic chemistry'. Mentions relativity.
Pershina (1998ab)	Hydrolysis of Group 5 cations in HCl: Nb,Ta,Pa,Db(E105).
Pershina et al. (1998)	Electronic structure of the transactinides.
Pyykkö et al. (1998); Labzowsky et al.(1999b)	Estimated valence-electron Lamb shifts for Li-E119, Cu-E111. About -1% of kinetic Dirac shifts for large Z. QED in chemistry about -1% of relativity in chemistry, for large Z.
Schwerdtfeger and Seth (1998)	Relativistic effects in superheavy elements.
Seth (1998)	Quantum chemistry of superheavy elements. Thesis.
Seth et al. (1998a)	Coinage metal fluoride anions for Cu-E111. E111 has the most stable +5 oxidation state.
Seth et al. (1998b)	Stability of oxidation state +4 in Group 14 (C-E114).
Söderlind (1998)	Theory of the crystal structures of Ce, early An. Review.
Autschbach (1999)	Trends of relativistic effects.
Cotton et al. (1999)	Inorganic chemistry textbook.
Fröhlich and Frenking (1999)	Bonding in transition-metal complexes. Carbonyls, carbenes, π-bonded systems, dihydrogen complexes.
Greiner and Gupta (1999)	Edited book on superheavy elements.
Han and Lee (1999)	SO effects and heavy RgF_n; n=2,4. Stabilization. $(E118)F_4$ obtains a T_d minimum due to SO.
Kaldor and Eliav (1999)	High-accuracy calculations for heavy and superheavy elements.
Kaltsoyannis and Scott (1999)	Textbook on f elements. Mentions relativity.
Kaupp (1999b)	Relationships between π bonding, electronegativity and bond angles in high-valent transition metal complexes. Bent's rule less valid for TM than for main-group elements.
Kedziora et al. (1999)	Relativistic effects on atomization energies. 148 species in Pople's G2/97 test set.
Kratz (1999)	Chemistry of the transactinides.
Leidler and Meiser (1999)	Physical chemistry textbook. Mentions relativistic effects.
W.-J. Liu and van Wüllen (1999)	MX; X=H,F-Br,O,Au. M_2; M=Au,E111. SO effects. Large atomic SO contributions due to E111 d^9s^2 ground state.
Mikheev and Rumer (1999)	Stabilization of Ln(II), An(II) in solutions, melts and clusters. Review.
Nash and Bursten (1999abc)	SO effects make $(118)F_4$ T_d, unlike D_{4h} XeF_4, RnF_4.
Nash and Bursten (1999d)	XH; X=Br-E117. $7p8s$ hybridization! Involves $7p_{3/2}$.
W. Paulus et al. (1999); Pershina and Bastug (1999)	Db(E105) chemistry in aqueous solution. Results lie between Nb and Ta.
Pershina and Fricke (1999)	Electronic structure and chemistry of the heaviest elements.
Pershina et al. (1999)	Redox potentials in acid solutions estimated for Cr-Sg.
Pettersson et al. (1999b)	New rare-gas-containing neutral molecules. Review.
Quiney et al. (1999)	Ab initio relativistic quantum chemistry.

Reference	Comments
Richardson et al. (1999ab)	HMOOH, MeMOOH isomers; M=C-Pb. Shift from M(IV) to M(II) in Group 14.
Schreckenbach et al. (1999)	DFT calculations on actinide compounds.
Seo and Hoffmann (1999)	Structures of solid elements P-Bi. Role of $s-p$ mixing.
Seth et al. (1999b)	Bonding trends in Group 13 (B-E113). MX_n; n=1,3,5. The (E113)X_3 are T-shaped, not D_{3h}. The $6d$ is involved.
Volkova and Magarill (1999)	Formation of polyatomic cations of mercury.
Watson et al. (1999)	The stereochemically active Pb(II) lone pair in solid α-PbO has $6s-2p$ hybridization.

Many of the papers in the following Table 9.2 also give data on relativistic changes of the force constant k_2 or the dissociation energy, D_e. C is the relativistic bond-length contraction, $C = R_{NR} - R_R$.

Table 9.2: Bond lengths, bond angles and potential-energy surfaces.

Reference	Comments
Barnes et al. (1993)	CO. C 0.013 pm. $\Delta\omega_e$ -1.3 cm^{-1}.
Bastug et al. (1993)	Au_2. DS (α=0.7) C 20.6 pm.
Dyall (1993a)	MO; M=Ge-Pb
Dyall (1993b)	PtH, PtH^+, PtH_2. PtH^+ C -2.5 pm. DF/HF.
Matsuoka et al. (1993)	PbO. C.
Schwerdtfeger and Ischtwan (1993)	TlX, TlX_3; X=F-I.
Bauschlicher et al. (1994)	AlCu C 4.2 pm. D_0 increase 0.225 eV.
Kaupp and von Schnering (1994a)	HgX_2; X=F-I, H. C.
Kaupp and von Schnering (1994c)	Solid HgF_2.
J. M. L. Martin and Taylor (1994)	HF. C -0.005 pm.
Park and Almlöf (1994)	Pt_2, MH,M_2; M=Ag,Au. Effect of two-electron DK terms.
Pisani and Clementi (1994b)	H_2E; E=O-Po. Bond-angle decrease for Po -1.66°, C 1.8 pm. DF/HF.
Pou-Amérigo et al. (1994)	CuH, NiH. PT relativity.
Schwerdtfeger and Bowmaker (1994)	MCO; M=Cu-Au.
Schwerdtfeger et al. (1994a)	MX_3; M=N-Bi; X=F-I. Inversion barrier.
Schwerdtfeger and Hunt (1999)	T-shaped transition state found for BiF_3.
Collins et al. (1995)	MH, M=Cu-Au. C at DF and DK level compared.
Schwerdtfeger (1995)	AuCl. R/NR for HF - QCISD(T).
Schwerdtfeger et al. (1995b)	AuF, AuF^+, AuF_2, Au_2F_2.
van Wüllen (1995,1996b)	C for carbonyls of Cr-W, Fe-Os, Ni-Pt.
S. G. Wang et al. (1995)	LnO; Ln=La ... Yb. YbF.
S. G. Wang and Schwarz (1995a)	LnH, LnF, LnO; Ln=La,Gd,Yb,Lu. C.
S. G. Wang and Schwarz (1995b)	MO, MH_4, MCl_4; M=C-Pb.
Saue et al. (1996)	XH; X=I,At,E117. DF/HF. C 0.6, -0.3, -12.9 pm, respectively.
Schwerdtfeger (1996)	Geometries of XF_3; X=Cl-At. Large bond angle effect.
Seth et al. (1996a)	HBr.
Seth et al. (1996b)	MH; M=Cu-E111. C.
Urban and Sadlej (1996)	C for AlM; M=Cu-Au. DK.
van Lenthe et al. (1996b)	SO effects on closed-shell diatomics. HI, ... Bi_2.
Visscher and Dyall (1996)	X_2; X=F-At. DF to DF+CCSD(T). C.

Reference	Comments
Visscher et al. (1996b)	HX; X=F-At. Up to CCSD(T). R/NR. C.
Barysz and Urban (1997)	BCu, BAg, BAu. C = 4.5, 16, 32.5 pm, respectively, at CASPT2 level.
D.-D. Dai and Li (1997)	Diatomic EuCh; Ch=O-Te. Small C (1-2 pm).
de Jong et al. (1997)	I_2.
Geipel and Hess (1997)	DK approach for solids (in crystal HF). Ag, AgX; X=F-Br. Bond contraction. Metal stabilized, salts destabilized by relativity.
Küchle et al. (1997)	Lanthanide and actinide contractions. Depend on the ligand (H,F,O). 6-11 pm for Ln, 11-17 pm for An. At NR level, expansion for the MO monoxides.
Laerdahl et al. (1997a)	MF; M=Cu-Au. C.
M.-S. Liao and Schwarz (1997a)	$[XMX]^{3-}$; M=Cu-Au; X=O-Se in crystal field. C.
W.-J. Liu et al. (1997b)	LnO, LnS; Ln=Eu,Yb. C.
Saue et al. (1997)	CsAu. DF/HF. C=41 pm.
Watanabe and Matsuoka (1997)	ThO. C -7.1 pm. DF/HF.
Barysz and Papadopoulos (1998)	NiH_2 X $^1A_1$ C 0.79 pm.
Barysz and Pyykkö (1998)	AuX^+; X=Be,Mg,C,Si. C 38.5, 31.2, 51.0 and 34.2 pm, respectively, at CASPT2 level.
Császár et al. (1998); Tarczay et al. (1999)	Potential-energy surface for water. The barrier to linearity. Relativity beats non-Born-Oppenheimer.
de Jong et al. (1998)	C for interhalogens up to IBr. HF to CCSD(T). All slightly negative.
Iliaš et al. (1998)	MF; M=Cu-Au. C, up to DK-CCSD(T) level.
H.-S. Lee et al. (1998)	SO effects on bonding in AuH,Au_2,TlH,Tl_2.
M.-S. Liao and Zhang (1998a)	RgX_n; Rg=Kr,Xe,Rn; X=F,Cl. Small C.
Malli and Styszyński (1998)	$RfCl_4$. C 6.7 pm. DF.
H. Müller et al. (1998)	HF at CCSDT1-r_{12} level. Effect on ω_e 23 cm^{-1}.
Quiney et al. (1998a)	TlF. DF/HF.
Seth et al. (1998a)	MF_n^-; n=2,4,6; M=Cu-E111. C at MP2 level.
Wahlgren et al. (1998)	Au_2 C as test of one-centre DK approximation.
Nash and Bursten (1999e)	$M(CO)_6$; M=Cr-W,U,Sg. Covalent radius for Sg 4 pm larger than for Mo or W.
Suzumura et al. (1999)	M_2, MH, MCl; M=Cu-Au. R/NR.
Turski (1999)	SiM; M=Cu-Au. C.

Table 9.3: Magnetic resonance parameters.

Reference	Comments
Ham (1965)	Dynamical Jahn-Teller effect in ESR. Partial quenching of SO.
Smelyansky et al. (1993)	Conduction-electron g-factors in noble metals.
Van de Walle and Blöchl (1993)	Hyperfine parameters in solids. Includes SR, uses δ-function FC term. PP.
Du and Li (1994)	Contribution of ligand SO to g-tensors in VX_2; X=Cl,Br.
Markendorf et al. (1994)	Hcp TM ($3d-5d$, Sc,...,Os). NMR spin-lattice relaxation.
Belanzoni et al. (1995)	g-Tensor, hfs of TiF_3.
Bündgen et al. (1995)	g-tensors in diatomic molecules. NO, O_2, SO.
Endo et al. (1995)	Si and C NMR shifts in SiX_4, $CH_{4-n}X_n$; X=Cl-I; n=1-4. PM3+SO.
Hota et al. (1995)	Solid PbTe. ^{207}Pb NMR shifts including SO effects. A 2% downfield effect via the 6s orbital.

Reference	Comments
Kaupp et al. (1995a)	Ligand NMR shifts in NMR complexes.
Kaupp et al. (1995b)	^{17}O NMR shifts in MO_4^q TM complexes.
Lushington et al. (1995); Lushington and Grein (1996)	Ab initio studies of g tensors on 2nd-row . molecules.
Nakatsuji et al. (1995a)	SO effects on NMR shifts. Si shifts in SiX_4; X=F-I, $SiXI_3$; X=Cl,Br. SO PP on X.
Nakatsuji et al. (1995b)	UHF PT method for SO effects on NMR shifts. 1-electron SO Hamiltonian only. HX, CH_3X; X=F-I. ^{1}H and ^{13}C NMR shifts.
Takashima et al. (1995)	MX_4^-; M=Ga-In; X=Cl-I. Ga, In NMR shifts. PT.
Willatzen et al. (1995)	II-VI zinc blende materials. SO parameters and electron g-factor.
Ballard et al. (1996)	Proton NMR shifts in HX, X=F-I.
Bastug et al. (1996)	Diamagnetic shielding for ^{209}Bi in $Bi(NO_3)_3$, Bi^{3+}. Almost equal. Lamb wrong. Recall Feiock and Johnson (1968).
Battocletti et al. (1996)	Influence of gradient corrections on M1 hfs in ferromagnetic Fe, Co, Ni.
Fowler et al. (1996)	EFG in BrCl. DK.
Fukui et al. (1996)	Relativistic effects in NMR shielding. Lowest order.
Hada et al. (1996)	^{183}W NMR shielding in WX_6; X=F,Cl, WO_4^{2-}. DK.
Hemmingsen and Ryde (1996)	EFG in Cd complexes.
Kaneko et al. (1996)	^{119}Sn NMR shifts in SnH_4, tin tetrahalides. PT SO. FC term dominates the shift.
Kaupp (1996a)	$[MCp(CO)_4]^-$; M=Ti-Hf. ^{13}C NMR shifts.
Kaupp (1996b)	^{13}C and ^{17}O NMR shifts in $Fe_2(CO)_9$, $Rh_6(CO)_{16}$.
Kaupp (1996c)	$[M(CO)_5L]$; M=Cr-W; L=PH_3, PX_3 ^{31}P NMR shifts.
Kaupp (1996f)	$[M_nC(CO)_m]^q$; M=Fe,Rh,Os interstitial carbides. ^{13}C NMR shifts.
Kaupp et al. (1996a)	$M(CO)_6$; M=Cr-W. C and O NMR shifts.
Kellö and Sadlej (1996b)	HX; X=Cl-I. Halogen Q.
Kutzelnigg et al. (1996)	IGLO method for NMR shift tensors. Review.
Malkin et al. (1996)	HX, CH_nX_{4-n}; X=F-I. SO-induced ^{1}H, ^{13}C NMR shifts.
Nakatsuji et al. (1996a)	HgX_2; X=Cl-I. ^{199}Hg NMR shifts. 1-electron SO only, FC operator on Hg.
Nakatsuji et al. (1996b)	AlX_4^-; X=H,F-I. ^{27}Al NMR shifts.
Ruiz-Morales et al. (1996)	$W(CO)_6$. C and O NMR shifts. SR/NR DFT.
Schreckenbach and Ziegler (1996)	DFT calculations of NMR shifts. (NR.)
K. Schwarz et al. (1996)	EFG calculations on solid borides. MB_2; M=Ti...Ta. MB_6; M=Ca-Ba.
Ehlers et al. (1997)	^{13}C shifts in $M(CO)_6^n$, M=Cr→Fe, Tc→Ru, Hf→Ir.
J. A. González et al. (1997)	NMR ^1J coupling constants in Me_3XY; X=C-Pb; Y=F,Cl. MNDO-level correlated approach.
Havlas and Michl (1997,1998, 1999); Havlas et al. (1998)	Zero-field splittings in organic biradicals.
Havlin et al. (1997)	^{13}C shielding tensors in metal-olefin complexes.
Kaupp et al. (1997a)	CX_3^+; X=F-I. ^{13}C NMR shifts.
Kaupp et al. (1997b)	^{17}O NMR shifts in MO_4; M=Fe-Os, MnO_4^-; M=Mn-Re, MO_4^{2-}; M=Cr-W.
Kirpekar et al. (1997)	Spin-spin coupling in XH_4; X=C-Sn. SO corrections only, no SR corrections. Found small.

Reference	Comments
Nakatsuji et al. (1997b)	TiX_4; X=F-I. Ti NMR shift. NbX_6^-, $NbCl_5X^-$; X=F-I. Nb NMR shift.
Oja and Lounasmaa (1997)	Nuclear magnetic ordering of simple metals. Covers theory of nuclear spin-spin coupling.
Pyykkö and Seth (1997)	H-like and DF-level relativistic correction factors for nuclear quadrupole coupling. Discusses 'SO tilting'.
Quiney et al. (1997)	Relativistic calculation of EM properties of molecules.
Ruiz-Morales et al. (1997)	^{125}Te NMR shifts. SR DFT.
Sasaki et al. (1997)	SO-induced electron-spin polarization in donor-acceptor complexes containing heavy halogen atoms. ESR.
Schreckenbach and Ziegler (1997)	SR DFT calculations of NMR shifts. Method described. ^{17}O shifts in MO_4^{n-}; M=Cr-W,...Os. $M(CO)_6$; M=Cr-W.
Svane et al. (1997)	Hfs parameters in tin compounds. $Q(^{119}\mathrm{Sn}(24\ \mathrm{keV};3/2+))$ obtained.
Vaara and Hiltunen (1997)	CD_3X; X=F-I. Deuterium EFG. PP.
van Lenthe et al. (1997)	ZORA calculations of molecular g-tensors.
Bruna and Grein (1998)	g-tensors of O_3^-, O_3Na, O_3Na.
Fukui and Baba (1998)	NMR shielding at no-pair level.
Ishikawa et al. (1998)	DF finite-field theory of NMR shielding. Applications on He-Xe, H_2, HF, HCl.
Kaupp and Malkina (1998)	$CH_n(HgX)_{4-n}$; X=Cl,CN; n=0-4. RHgH; R=Me, Et,.. ^{13}C and ^{1}H NMR shifts.
Kaupp et al. (1998a)	NMR of transition-metal compounds.
Kaupp et al. (1998b)	A simple interpretation for SO-induced NMR shifts, analogous to FC spin-spin coupling. Applied on iodo-organic compounds. ^{1}H and ^{13}C shifts.
Kellö and Sadlej (1998a)	Picture-change effects for EFG. HI, HAt as examples.
Kellö and Sadlej (1998b)	Q(K) from KF, KCl.
Lobayan and Aucar (1998ab)	NMR spin-spin coupling constants within PM3 parametrization, CLOPPA scheme. As-Bi, Ga-Tl, Si-Pb.
Malkina et al. (1998)	HX, CH_3X; X=F-I. SO-induced ^{1}H, ^{13}C NMR shifts. Importance of two-electron SO terms.
Minaev et al. (1998)	R-dependence of the SO-induced ^{1}H NMR shift in HX; X=Cl-I.
Neese and Solomon (1998)	INDO/S-CI for ZFS and g-factors in TM complexes. $FeCl_4^-$ as example. Results compared with BP PT ab initio ones.
Patnaik et al. (1998)	PbTe. Nuclear spin-spin coupling. δ-function FC term used?
Pernpointner and Schwerdtfeger (1998)	GaF. Q(Ga) obtained.
Pernpointner et al. (1998a)	CsF. Q(Cs) obtained. DK CCSD(T).
Pernpointner et al. (1998b)	CuF. PCNQM (point-charge nuclear quadrupole moment model) developed. DF or DK + CCSD(T).
Quiney et al. (1998b)	Hfs in YbF.
Quiney et al. (1998c)	NMR shielding in H_2O. DF.
Schreckenbach and Ziegler (1998)	DFT calculation of NMR shifts and ESR g-tensors. Review.
Soldner et al. (1998a)	EFG calculations for isolated molecules using WIEN95. Examples: $CdCl_2$, HgX_2; X=F,Cl.
Soldner et al. (1998b)	Hg EFG for mercaptides $Hg(SR)_2$; R=Me,Et,Pr.
Vaara et al. (1998)	Quadratic response calculation of SO contributions

Reference	Comments
	to NMR shift tensors. HX, CH_3X; X=F-I.
van Lenthe et al. (1998)	ZORA DFT calculations of g-tensors, hfs, in M_5, M_7, M,M'=Cu-Au.
Visscher et al. (1998)	EFG in HX; X=Cl-I. MP2 to CCSD(T). R/NR.
Wolff and Ziegler (1998)	DFT-GIAO NMR shifts including SO. HX, CH_3X, TM carbonyl ^{13}C shifts; TM=Hf-Hg.
Yamaguchi and Miyagi (1998)	Molecular solid I_2 under pressure. EFG and Mössbauer isomer shift.
Baba and Fukui (1999)	Gauge-origin-independent relativistic effects on NMR shifts.
Bruna and Grein (1999)	g-tensors for X_2^-, MX_2, $M_2X_2^+$; M=Li,Na; X=F,Cl.
Bühl (1999)	^{95}Mo NMR chemical shifts.
Bühl et al. (1999)	Review on DFT calculations on NMR shifts.
Cromp et al. (1999)	NMR chemical shifts in DFT. SO, rovibration effects. HBr.
Ebert et al. (1999a)	Fully relativistic description of static M1 hfs in magnetic and nonmagnetic solids. Knight shifts of 4d elements.
Hada et al. (1999)	HX;X=H,F-I. Proton NMR shifts.
Helgaker et al. (1999)	Review on ab initio calculations of NMR shielding and spin-spin coupling tensors.
Hemmingsen et al. (1999)	EFG in β-$Cd(OH)_2$. SO effect small.
Kaupp et al. (1999a)	PI_4^+ ^{31}P NMR shifts due to SO.
Kaupp et al. (1999b)	CF_3IF_n; n=0,2,4,6. ^{13}C and ^{19}F NMR shifts.
Kellö and Sadlej (1999a)	Q(Ge) from GeO, GeS.
Kellö and Sadlej (1999b)	Q(Rb) from RbF, RbCl. Summary of alkali Q.
Kellö et al. (1999)	Q(Al) from AlF, AlCl.
Kutzelnigg (1999b)	Relativistic corrections to magnetic properties. DPT.
W.-J. Li et al. (1999ab)	Introduce CI to A. J. Stone's $(1963)^{2777}$ theory of the g-matrix. Applications on $[MOX_n]^{m-}$; M=V,Cr,Mo; X=F-Br.
Moore (1999)	Magnetic shielding (NMR shift) for H-like Dirac atom. Closed-form expressions.
Patchkovskii and Ziegler (1999)	d^1 systems MEX_4^{z-}; M=V,Cr-W,Tc-Re; E=O,N; X=F-Br. g-tensors. DFT.
Pyper (1999ab)	Nuclear shielding in one-electron atoms.
Rodriguez-Fortea et al. (1999)	$WO_nS_{4-n}^{2-}$; n=0-4, WX_6; X=F,Cl,CO. ^{183}W NMR shifts. Me_3PbX; X=Cl-I, -OMe, -SMe, -SeMe, $-NEt_2$. PbX_4; X=Cl-I. ^{207}Pb NMR shifts. ZORA relativity. For W, paramagnetic contributions dominate. For Pb, SO-induced FC contributions dominate.
Schwerdtfeger et al. (1999)	EFG in HCl and CuCl. Accuracy of the DFT approach. DK.
Seth et al. (1999a)	EFG in HCl, MCl; M=Li-K. DK.
Vaara et al. (1999a)	HX, CH_3X; X=F-I. H_2X; X=O-Te. H, C and X NMR shift tensors. 2nd- and 3rd-order SO effects. SOO included.
Vaara et al. (1999b)	HX; X=F-I. H_2X; X=O-Te. NMR spin-spin coupling. 2nd- and 3rd-order SO effects. SOO.
Visscher et al. (1999)	HX; X=F-I. NMR shielding and spin-spin coupling.
Wolff et al. (1999)	NMR shifts using ZORA and DFT. ^{199}Hg in LHgL'. Solvent shifts using simple models.

Table 9.4: Electric dipole moments and molecular charge distributions. For electric field gradients, see previous table.

Reference	Comments
Dolg et al. (1993a)	Dipole moment of PbO. Both SR and SO effects included. The SO must be treated at correlated level. AE vs. PP tested.
Dyall (1993a)	MO; M=Ge-Pb. Dipole moment at DF/HF level.
Kellö and Sadlej (1993)	MO, MS; M=Si-Pb. Dipole moments. PT relativity.
Perera and Bartlett (1993)	Dipole moments of interhalogens, up to IBr. PT relativity, CCSD correlation.
Reinisch and Bross (1993)	Relativistic effects on the Compton profile of polycrystalline gold.
Pou-Amérigo et al. (1994)	Dipole moments of MH; M=Ni, Cu. PT relativity.
Schwerdtfeger and Bowmaker (1994)	MCO; M=Cu-Au. Dipole polarizabilities.
Kellö and Sadlej (1995b)	Dipole moments of MH; M=Cu-Au. PT relativity.
Kellö and Sadlej (1995c)	Electric properties of CuAg, CuAu, AgAu. PT relativity. Sign of CuAu dipole moment changed by R.
Schwerdtfeger (1995)	AuCl. R/NR dipole moment and polarizability for HF - QCISD(T).
Urban and Sadlej (1995)	MM'; M,M'=Li-Rb. Electric properties. PT.
Kellö and Sadlej (1996a); Kellö et al. (1996)	Dipole moments of MH; M=Cu-Au. SR DK CCSD(T). R/NR.
Urban and Sadlej (1996)	Electric properties for AlM; M=Cu-Au. DK.
D.-D. Dai and Li (1997)	Diatomic EuCh; Ch=O-Te. Dipole moment decrease.
de Jong et al. (1998)	Interhalogens up to IBr. HF to CCSD(T). Both μ and Θ.
Ilıaš et al. (1998)	MF; M=Cu-Au. Dip. mom., up to DK-CCSD(T) level.
Kellö et al. (1998)	MO, MS; M=Si-Pb. Dipole moments. DK relativity. For PbO a large SO effect found.
Miadoková et al. (1999)	Electric properties of MF; M=K-Fr. NR/PT/DK.
Raptis et al. (1999)	Electric properties of MS; M=Zn-Hg. DK/NR.
Suzumura et al. (1999)	MH, MCl; M=Cu-Au. Dipole moments. SR/NR DFT.
Turski (1999)	SiM; M=Cu-Au. Dipole moment R/NR.

Table 9.5: Molecular energy levels and energy transfer.

Reference	Comments
Minaev et al. (1993)	Effect of intermolecular interaction on forbidden transitions of O_2. SO.
Minaev et al. (1995)	Singlet-triplet transitions of N_2.
Ågren et al. (1996)	Review on SO effects, handled with response theory. Predissociation, triplet bands, phosphorescence, external heavy-atom effects.
Minaev et al. (1996)	Magnetic phosphorescence of O_2 b $^1\Sigma_g^+$ - X $^3\Sigma_g^-$ red atmospheric emission band.

The following Table 9.6 gives available results on relativistic – especially spin-orbit – effects on chemical reactions. For further examples, see Table 7.10 and look for the symbol '+'.

Table 9.6: Relativistic effects on chemical reactions.

Reference	Comments
Minaev (1983)	SO effects in molecular spectroscopy and chemical kinetics. Thesis.
Yarkony (1992)	Spin-forbidden chemistry within BP approximation. Review.
Alexander et al. (1993)	SO branching in the photofragmentation of HCl.
Chang and Yarkony (1993)	Spin-forbidden processes in $N_2O \rightarrow N_2+O(^3P)$.
L. Li et al. (1993)	Experimental reactions of M_2; M=Cu-Au with O_2, N_2O, N_2, H_2, CH_4, CO, CO_2, C_2H_4 in the gas phase. Au_2 anomalous. Reasons discussed.
Minaev and Lunell (1993)	Classification of SO effects in organic reactions.
Daniel et al. (1995)	SO-induced radiationless transitions in $HCo(CO)_4$.
Knuts et al. (1995)	SO effects in oxirane ring opening.
Minaev and Ågren (1995, 1996)	Reviews on SO-induced chemical reactivity and 'spin-catalysis'.
Riad Manaa (1995)	SH (A $^2\Sigma^+$). Fragmentation. SO.
Su (1995a)	Photochemical rearrangement of 3-substituted cyclopropenes to cyclopentadienes. SO.
Su (1995b)	Photorearrangements of cyclohexadienes.
Su (1995c)	Photochemical rearrangement of vinylcyclopropanes to cyclopentenes. SO. Triplet excited state, singlet ground state.
Visscher and Dyall (1995)	$H+Cl_2 \rightarrow HCl+Cl$. $Cl+HCl \rightarrow ClH+Cl$. Rel. effects on reaction energy. DF+MP2/DK/NR.
Ågren et al. (1996)	Review on spin catalysis.
Böckmann et al. (1996)	SO coupling in organic molecules. MNDOC-CI. Triplet-state reactivity.
Brouder et al. (1996)	X-ray magnetic circular dichroism. Fe K-edge.
Musaev and Morokuma (1996)	Potential-energy surfaces of TM-catalyzed chemical reactions.
Su (1996a)	SO coupling and triplet carbenic addition chemistry.
Su (1996b)	SO coupling in photochemical reaarangements of α,β-unsaturated cyclic ketones.
Su (1996c)	SO coupling in oxadi-π-methane rearrangements and related photochemical reactions.
Yarkony (1996)	CH (a $^4\Sigma^-$) + CO (X $^1\Sigma^+$). Surface of intersection, SO interaction and Kramers degeneracy.
Danovich and Shaik (1997)	SO coupling in oxidative addition of $FeO^+ + H_2$.
Alexander et al. (1998)	SO effects on $F(^2P) + H_2$.
Aquilanti et al. (1998)	SO effects on $F + H_2$.
Danovich et al. (1998)	SO effects in twist and pyramidalization of ethene. BP + MRCI study.
Kaledin et al. (1998)	$I(^2P_{3/2})+O_2(a\ ^1\Delta_g) \leftrightarrow I(^2P_{1/2})+O_2(X\ ^3\Sigma_g^-)$. SO.
Minaev and Ågren (1998)	SO coupling in oxygen-containing diradicals. Reaction paths. MNDO CI.
Aoiz et al. (1999)	SO effects for $F + H_2 \rightarrow HF + H$.
Daniel et al. (1999)	$M(H)(CO)_3$(H-DAB); M=Mn,Re; H-DAB = 1,4-Diaza-1,3-butadiene. SO effects on the M-H bond homolysis.
Honvault and Launay (1999)	SO corrections to $F+D_2 \rightarrow DF+D$.

Reference	Comments
S.-H. Lee and Liu (1999)	SO reactivity of Cl atom: In $Cl(^2P)+H_2 \rightarrow HCl+H$ the excited $Cl^*(^2P_{1/2})$ state is more reactive. Exp.
Riad Manaa (1999)	Photodissociation of NaK.

Chapter 10

Appendix

Table 10.1: List of acronyms and symbols.

Symbol	Meaning
A	Magnetic vector potential.
AE	All-electron (as contrasted to PP).
AMFI	Atomic mean field spin-orbit operator.
An	Actinide.
B	Magnetic field.
BP	Breit-Pauli.
BW	Bohr-Weisskopf effect.
CC	Coupled-cluster (method).
CCSD	Coupled clusters with single and double excitations.
COT	Cyclo-octatetraene, C_8H_8.
Cp	Cyclopentadiene, C_5H_5.
Cp*	Pentamethylcyclopentadiene, $C_5(CH_3)_5$.
nD	n-dimensional.
DC	Dirac-Coulomb.
DCB	Dirac-Coulomb-Breit (Hamiltonian).
DF	Dirac-Fock (='Dirac-Hartree-Fock').
DFB	Dirac-Fock-Breit.
DFT	Density functional theory.
DIM	Diatomics-in-molecule (a semiempirical model).
DPT	Direct perturbation theory.
DQCC	Deuteron quadrupole coupling constant.
DSW	Dirac Scattered-Wave.
DVM	Discrete variational method.
EA	Electron affinity.
ECP	Effective core potential (=PP).
EFG	Electric field gradient.
EM	Electromagnetic.
ESC	Elimination of small component.
Et	Ethyl, $-CH_2CH_3$.
EXAFS	Extended x-ray absorption fine structure.
FC	Fermi contact term.
FEM	Finite-element method.
FS	Fine structure.
FW	Foldy-Wouthuysen[1019] (-Tani[6210,6211]) transformation.
GGA	Generalized gradient approximation.
GTO	Gaussian type orbital.
GUGA	Graphical unitary group approach.
h_D	One-electron Dirac Hamiltonian.
Hfs	Hyperfine structure.
INDO	Intermediate neglect of differential overlap.
	A semiempirical MO method.
IP	Ionization potential.
j	Current density.
KG	Klein-Gordon (equation).
LAPW	Linearized augmented plane wave method.
LCAO	Linear Combination of Atomic Orbitals.
LDA	Local density approximation (in DFT).
LMTO	Linear muffin-tin orbital.

Symbol	Meaning
Ln	Lanthanide.
μ	Molecular dipole moment.
mb	Millibarn (10^{-31} m^2).
MBPT	Many-body perturbation theory.
MC	Monte-Carlo.
MCDF	Multiconfiguration Dirac-Fock.
Me	Methyl, -CH_3.
MP	Model potential (with nodes).
MPn	Møller-Plesset PT of order n.
MQDT	Multichannel quantum defect theory.
MRCI	Multireference CI.
MXD	Magnetic x-ray dichroism.
NR	Non-relativistic.
PES	Photoelectron spectrum.
Ph	Phenyl, -C_6H_5.
PP	Pseudopotential (=ECP).
PT	Perturbation theory.
π	$\mathbf{p} - e\mathbf{A}$.
Q	Nuclear quadrupole moment.
QDT	Quantum Defect Theory.
QED	Quantum Electrodynamics.
QM	Quantum Mechanics.
QMC	Quantum Monte Carlo.
R	Interatomic distance.
R	Relativistic.
RA	Regular Approximation.
RASCI	Restricted Active Space Configuration Interaction.
RESC	Relativistic scheme by Eliminating Small Components.
REX	Relativistic Extended Hückel.
RI	Resolution-of-the-identity, $\sum_n \|n><n\| = 1$.
ρ	Charge density.
RRPA	Relativistic random phase approximation.
SE	Self energy.
SO	Spin-orbit.
SOO	Spin-other-orbit.
SR	Scalar relativistic (spin-orbit averaged, 'quasirelativistic').
SW	Scattered wave (=multiple-scattering method, MS Xα).
Θ	Molecular quadrupole moment.
TB	Tight binding (= EHT for crystals).
TF	Thomas-Fermi.
TM	Transition metal.
TP	Transition probability.
UHF	Unrestricted Hartree-Fock (different orbitals for different spins).
VP	Vacuum polarization.
WB	Wood-Boring Hamiltonian (Wood and Boring 1978)[3037].
WKB	Wentzel-Kramers-Brillouin approximation, semiclassical ($\hbar \to 0$) approximation.
XAS	X-ray absorption spectra.
XMCD	X-ray magnetic circular dichroism.

Symbol	Meaning
Z	Nuclear charge.
ZFS	Zero-field splitting.
ZORA	Zeroth-order regular approximation.

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