Publications by Dage Sundholm

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A: Peer-reviewed scientific articles

266. M. Orozco-Ic, J. Barroso, N. D. Charistos, R. Islas, A. Muñoz-Castro, D. Sundholm, G. Merino, "The magnetic response of corannulene through its bowl-to-bowl inversion", Chem. Eur. J. (2021) (submitted).

265. M. Dimitrova, S. Lehtola, D. Sundholm, T. Helgaker, S. Stopkowicz, "Small hydrocarbons in strong magnetic fields: CH and CH_2", (2021) (manuscript).

264. M. Orozco-Ic, M. Dimitrova, J. Barroso, D. Sundholm, G. Merino, "Magnetically induced ring-current strengths of planar and non-planar molecules: New insights from the pseudo-π model", (2021) (manuscript)

263. K. Nordlund, M. Hori, D. Sundholm, "Strong nuclear scattering effects on antiproton transmission through foils", Phys. Rev. A (2021) (manuscript).

262. M. Dimitrova, D. Sundholm, "Current density, current-density pathways and molecular aromaticity", Chapter 5 in Aromaticity: Modern Computational Methods and Applications, Ed. I. Fernández López, Elsevier (2021) DOI: 10.1016/C2019-0-04193-3

261. D. Sundholm, H. Fliegl, "Aromatic Pathways in Porphyrinoids by Magnetically Induced Ring Currents", Handbook of Porphyrin Science, Vol. 46, Eds K. M. Kadish, K. M. Smith and R. Guilard, World Scientific (2021) (in press).

260. R. R. Valiev, R. T. Nasibullin, V. N. Cherepanov, A. Kurtzevich, D. Sundholm, and T. Kurtén, "Fast estimation of the internal conversion rate constant in photophysical applications", Phys. Chem. Chem. Phys., 23 (2021) 6344-6348. DOI: 10.1039/D1CP00257K

259. R. Kumar Jinger, H. Fliegl, R. Bast, M. Dimitrova, S. Lehtola, D. Sundholm, "Spatial contributions to NMR chemical shifts", J. Phys. Chem. A 125 (2021) 1778-1786. DOI: 10.1021/acs.jpca.0c10884

258. S. Lehtola, M. Dimitrova, H. Fliegl, D. Sundholm, "Benchmarking magnetizabilities with recent density functionals", J. Chem. Theory Comput. 17 (2021) 1457-1468. DOI: 10.1021/acs.jctc.0c01190

257. D. Casadio, S. Aikonen, A. Lenarda, M. Nieger, T. Hu, S. Taubert, D. Sundholm, M. Muuronen, T. Wirtanen, J. Helaja, "Divergent Carbocatalytic Routes in Oxidative Coupling of Benzofused Heteroaryl Dimers: A Mechanistic Update", Chem. Eur. J. 27 (2021) 2021, 5283-5291. DOI: 10.1002/chem.202005433

256. G. Baryshnikov, R. R. Valiev, R. Nasibullin, D. Sundholm, T. Kurtén, H. Ågren, The Aromaticity of Even Number Cyclo[n]carbons (n=6-100), J. Phys. Chem. A 124 (2020) 10849-10855. DOI: 10.1021/acs.jpca.0c09692

255. R. R. Valiev, L. I. Valiulina, H. Fliegl, D. Sundholm, "The effect of anion complexation on the aromatic properties of aromatic and antiaromatic porphyrinoids", New. J. Chem. 44 (2020) 20643-20650. DOI:10.1039/D0NJ04470A

254. R. R. Valiev, G. V. Baryshnikov, D. Sundholm, H. Ågren, B. F. Minaev, T. Kurtén, "First-principles calculations of anharmonic and deuteration effects on photophysical properties of polyacenes and porphyrinoids", Phys. Chem. Chem. Phys., 22 (2020), 22314-22323. DOI:10.1039/D0CP03231J (2020 PCCP HOT Articles)

253. J. M. López-de-Luzuriaga, M. Monge, M. E. Olmos, M. Rodrıguez-Castillo, I. Soldevilla, D. Sundholm, R. R. Valiev,"Perhalophenyl Three-coordinate Au(I) Complexes as TADF Emitters: A Photophysical Study from Experimental and Computational Viewpoints", Inorg. Chem. 59 (2020) 14236-14244. DOI:10.1021/acs.inorgchem.0c02018

252. R. R. Valiev, G. V. Baryshnikov, R. T. Nasibullin, D. Sundholm, H. Ågren, "When are antiaromatic molecules paramagnetic?", J. Phys. Chem. C 124 (2020) 21027-21035. DOI:10.1021/acs.jpcc.0c01559

251. M. Orozco-Ic, C. A. Celaya, D. Sundholm, "Calculations of magnetic response properties of tetrazines", RSC Advances 10 (2020) 18124-18130. DOI:10.1039/D0RA01641A

250. C. A. Celaya, M. Orozco-Ic, M. Dimitrova, L. N. Wirz, D. Sundholm, "A method for designing a novel class of gold-containing molecules", Chem. Commun. 56 (2020) 5433–5436. DOI:10.1039/D0CC01227K

249. J. Greiner, R. R. Valiev, D. Sundholm, "Photophysical properties of the triangular $[Au(HN{=}COH)]_3$ complex and its dimer", Phys. Chem. Chem. Phys. 22 (2020) 10314-10321. DOI:10.1039/D0CP01406K

248. L. F. Pašteka, T. Helgaker, T. Saue, D. Sundholm, H.-J. Werner, M. Hasanbulli, J. Major, P. Schwerdtfeger, "Atoms and molecules in soft confinement potentials", Mol. Phys. 118 (2020) e1730989. DOI:10.1080/00268976.2020.1730989

247. I. Benkyi, O. Staszewska-Krajewska, D. T. Gryko, M. Jaszuński, A. Stanger, D. Sundholm, "The interplay of aromaticity and antiaromaticity in N-doped nanographenes", J. Phys. Chem. A 124, (2020) 695-703. DOI: 10.1021/acs.jpca.9b11315

246. J. Greiner, D. Sundholm, "Calculation of Vibrationally Resolved Absorption and Fluorescence Spectra of the Rylenes", Phys. Chem. Chem. Phys. 22 (2020) 2379-2385. DOI: 10.1039/C9CP06089H; "Correction: Calculation of vibrationally resolved absorption and fluorescence spectra of the rylenes", Phys. Chem. Chem. Phys. 22 (2020) 4277-4277. DOI:10.1039/D0CP90033H

245. Y. Shao, Y. Mei, D. Sundholm, V. R. I. Kaila, "Benchmarking the performance of time-dependent density functional theory methods on biochromophores", J. Chem. Theory Comput. 16 (2020) 587-600. DOI: 10.1021/acs.jctc.9b00823.

244. G. Baryshnikov, R. R. Valiev, A. Kuklin, D. Sundholm, H. Ågren, "Cyclo[18]Carbon: Insight into Electronic Structure, Aromaticity and Surface Coupling", J. Phys. Chem. Letters 10 (2019) 6701-6705. DOI: 10.1021/acs.jpclett.9b02815

243. I. Benkyi, E. Tapavicza, H. Fliegl, D. Sundholm, "Calculation of vibrationally resolved absorption spectra of acenes and pyrene" Phys. Chem. Chem. Phys. 21 (2019) 21094-21103. DOI: 10.1039/C9CP04178H

242. K. Bartkowski, M. Dimitrova, P. J. Chmielewski, D. Sundholm, M. Pawlicki, "Aromatic and Antiaromatic Pathways in Triphyrin(2.1.1) Annelated with Benzo[b]heterocycles", Chem. Eur. J. 25 (2019) 15477-15482. DOI: 10.1002/chem.201903863 (2019 Hot Paper)

241. R. R. Valiev, V. N. Cherepanov, R. T. Nasibullin,V. Ya. Arthuhov, D. Sundholm, T. Kurtén, "Calculating rate constants for intersystem crossing and internal conversion in the Franck-Condon and Herzberg-Teller approximations" Phys. Chem. Chem. Phys. 21 (2019) 18495-18500. DOI: 10.1039/C9CP03183A. (2019 HOT PCCP article).

240. H. Rabaâ, M. Chiheb, A. L. Balch, D. Sundholm, "Predicting stable molecular structures for $(RNC)_2Au^IX$ complexes" Z. Anorg. Allgem. Chem. 645 (2019) 1127-1134. DOI:10.1002/zaac.201900134

239. R. R. Valiev, G. V. Baryshnikov, V. N. Cherepanov, D. Sundholm "Ab Initio Study of Phosphorescence of Hetero[8]circulenes", Russ. Phys. J. 62 (2019) 406-410. DOI: 10.1007/s11182-019-01727-7 (Translated from Izvestiya Vysshikh Uchebnykh Zavedenii, Fizika, No. 3, pp. 21-25, March, 2019.)

238. K. Reiter, F. Weigend, L. N. Wirz, M. Dimitrova, D. Sundholm, "Magnetically Induced Current Densities in Toroidal Carbon Nanotubes", J. Phys. Chem. C 123 (2019) 15354-15365. DOI: 10.1021/acs.jpcc.9b03769

237. S. Lehtola, M. Dimitrova, D. Sundholm, "Fully numerical electronic structure calculations on diatomic molecules in weak and strong magnetic fields", Mol. Phys. 114 (2020) e1597989. DOI:10.1080/00268976.2019.1597989

236. R. T. Nasibullin, R. R. Valiev, K. M. Faiskanova, E. V. Stepanova, V. N. Cherepanov, V. D. Filimonov, D. Sundholm, "Deacetylation of per-acetylated glycopyranosides: An overall pattern for acidic catalysis", Chem. Phys. Lett. 723 (2019) 123-127. DOI: 10.1016/j.cplett.2019.03.022

235. C. M. Suomivuori, H. Fliegl, E. B. Starikov, T. S. Balaban, V. R. I. Kaila, D. Sundholm, "Absorption Shifts of Diastereotopically Ligated Chlorophyll Dimers of Photosystem I", Phys. Chem. Chem. Phys. 21 (2019) 6851-6858. DOI: 10.1039/C9CP00616H (Hot PCCP paper 2019)

234. I. Benkyi, D. Sundholm, "Aromatic pathways in porphycene derivatives based on current-density calculations", J. Phys. Chem. A 123 (2019) 284-292. DOI: 10.1021/acs.jpca.8b10818

233. R. R. Valiev, G. V. Baryshnkiov, D. Sundholm, "Relations between the aromaticity and magnetic dipole transitions in the electronic spectra of hetero[8]circulenes", Phys. Chem. Chem. Phys. 20 (2018) 30239-30246. DOI: 10.1039/C8CP05694C

232. R. R. Valiev, A. K. Drozdova, P. V. Petunin, P. S. Postnikov, M. E. Trusova, V. N. Cherepanov, D. Sundholm, "The aromaticity of verdazyl radicals and their closed-shell charged species", New J. Chem. 42 (2018) 19987-19994. DOI: 10.1039/C8NJ04341H

231. D. Rico del Cerro, R. Mera-Adasme, A. W. T. King, J. E. Perea-Buceta, S. Heikkinen, T. Hase, D. Sundholm, K. Wähälä, "On the mechanism of the reactivity of 1,3-dialkylimidazolium salts under basic to acidic conditions: a combined kinetic and computational study", Angew. Chem. Int. Ed. 57 (2018) 11613-11617. DOI: 10.1002/anie.201805016

230. R. R. Valiev, H. Fliegl, D. Sundholm, "Bicycloaromaticity and Baird-type bicycloaromaticity of dithienothiophene-bridged [34]octaphyrins", Phys. Chem. Chem. Phys. 20 (2018) 17705-17713. DOI: 10.1039/C8CP03112F (Chosen as hot PCCP paper 2018)

229. P. Parkkinen, W. H. Xu, E. Solala, D. Sundholm, "Density Functional Theory under the Bubbles and Cube Numerical Framework", J. Chem. Theory Comput. 14 (2018) 4237-4245. DOI: 10.1021/acs.jctc.8b00456

228. C. Donsbach, K. Reiter, D. Sundholm, F. Weigend, S. Dehnen, "$[Hg_4Te_8(Te)_4]^{8-}$: An Electron-Rich Heavy Metal Porphyrinoid Embedded in a Lamellar Structure", Angew. Chem. Int. Ed. 57 (2018) 8770-8774. DOI: 10.1002/anie.201803233

227. R. R. Valiev, I. Benkyi, Y. Konyshev, H. Fliegl, D. Sundholm, "Computational studies of the aromatic and photophysical properties of expanded porphyrins", J. Phys. Chem. A 122 (2018) 4756-4767. DOI: 10.1021/acs.jpca.8b02311

226. E. Solala, P. Parkkinen, D. Sundholm, "Tensor decompositions for the bubbles and cube numerical framework" Comp. Phys. Commun. 232 (2018) 98-103. DOI:10.1016/j.cpc.2018.05.016

225. L. N. Wirz, M. Dimitrova, H. Fliegl, D. Sundholm, "Magnetically induced ring-current strengths in Möbius twisted annulenes", J. Phys. Chem. Lett. 9 (2018) 1627-1632. DOI: 10.1021/acs.jpclett.8b00440

224. R. R. Valiev, V. N. Cherepanov, G. V. Baryshnikov, D. Sundholm,"First-principles method for calculating the rate constants of internal-conversion and intersystem-crossing transitions", Phys. Chem. Chem. Phys. 20 (2018) 6121-6133. DOI: 10.1039/c7cp08703a

223. D. Sundholm, P. Pyykkö, "The argon nuclear quadrupole moments", Mol. Phys. 116 (2018) 1682-1686. DOI:10.1080/00268976.2018.1442938

222. H. Rabaâ, M. Omary, S. Taubert, D. Sundholm, "Insights into molecular structures and optical properties of stacked $[Au_3(RN{=}CR')_3]_n$ complexes", Inorg. Chem. 57 (2018) 718-730. DOI: 10.1021/acs.inorgchem.7b02593

221. H. Fliegl, R. R. Valiev, F. Pichierri, D. Sundholm, "Theoretical studies as a tool for understanding the aromatic character of porphyrinoid compounds", Chem. Modell. 14 (2018) 1-42. DOI: 10.1039/9781788010719-00001

220. M. Dimitrova, D. Sundholm, "The aromatic character of [10]annulenes and dicupra[10]-annulenes from current density calculations", Phys. Chem. Chem. Phys. 20 (2018) 1337-1346. DOI: 10.1039/C7CP07212K

219. K. Nordlund, D. Sundholm, P. Pyykkö, D. M. Zambrano, F. Djurabekova, "Nuclear stopping power of antiprotons", Phys. Rev. A 96 (2017) 042717(1-15). DOI: 10.1103/PhysRevA.96.042717

218. R. R. Valiev, H. Fliegl, D. Sundholm, "Optical and magnetic properties of antiaromatic porphyrinoids", Phys. Chem. Chem. Phys. 19 (2017) 25979-25988. doi:/10.1039/C7CP05460B

217. C. Kumar, H. Fliegl, D. Sundholm, "Relation Between Ring Currents and Hydrogenation Enthalpies for Assessing the Degree of Aromaticity", J. Phys. Chem. A, 121 (2017) 7282-7289. doi: 10.1021/acs.jpca.7b07607

216. F. Mendizabal, R. Mera-Adasme, D. Sundholm W. H. Xu, "Electronic and optical properties of metalloporphyrins of zinc on TiO_2 cluster in dye-sensitized solar-cells (DSSC). A quantum chemistry study", RSC Advances 7 (2017) 42677-42684. doi: 10.1039/c7ra08648b

215. R. R. Valiev, H. Fliegl, D. Sundholm, "Closed-shell paramagnetic porphyrinoids", Chem. Commun. 53 (2017) 9866-9869. doi: 10.1039/C7CC05232D

214. M. Dimitrova, H. Fliegl, D. Sundholm, "The influence of heteroatoms on the aromatic character and the current pathways of B_2N_2-dibenzo[a,e]pentalenes", Phys. Chem. Chem. Phys. 19 (2017) 20213-20223. doi: 10.1039/C7CP02964K

213. C. M. Suomivuori, A. P. Gamiz-Hernandez, D. Sundholm, V. R. I. Kaila, "Energetics and dynamics of a light-driven sodium-pumping rhodopsin", Proc. Natl. Acad. Sci. (USA) 114 (2017) 7043-7048. doi: 10.1073/pnas.1703625114

212. Y. J. Franzke, D. Sundholm, F. Weigend, "Calculations of current densities and aromatic pathways in cyclic porphyrin and isoporphyrin arrays", Phys. Chem. Chem. Phys. 19 (2017) 12794-12803. DOI: 10.1039/C7CP00624A

211. D. Sundholm, M. Rauhalahti, N. Özcan, R. Mera-Adasme, J. Kussmann, A. Luenser, C. Ochsenfeld, "Nuclear Magnetic Shieldings of Stacked Aromatic and Antiaromatic Molecules", J. Chem. Theory Comput. 13 (2017) 1952-1962.
DOI: 10.1021/acs.jctc.6b01250

210. M. Rauhalahti, S. Taubert, D. Sundholm, V. Liégeois, "Calculations of current densities for neutral and doubly charged persubstituted benzenes using effective core potentials", Phys. Chem. Chem. Phys. 19 (2017) 7124-7131. DOI: 10.1039/c7cp00194k

209. V. Molina, M. Rauhalahti, J. Hurtado, H. Fliegl, D. Sundholm, A. Muñoz-Castro, "Aromaticity introduced by antiferromagnetic ligand mediated metal-metal interactions. Insights from the induced magnetic response in $[Cu_6(dmPz)_6(OH)_6]$", Inorg. Chem. Front. 4 (2017) 986-993. DOI: 10.1039/C7QI00023E

208. P. Parkkinen, S. A. Losilla, E. Solala, E. A. Toivanen, W. H. Xu, D. Sundholm, "A Generalized Grid-Based Fast Multipole Method for Integrating Helmholtz Kernels", J. Chem. Theory Comput. 13 (2017) 654-665
DOI: 10.1021/acs.jctc.6b01207

207. P. Štěpánek, S. Coriani, J. Mareš, D. Sundholm, V. A. Ovchinnikov, J. Vaara, "Relation between molecular electronic structure and nuclear spin-induced circular dichroism", Sci. Rep. 7 (2017) 46617 doi: 10.1038/srep46617

206. E. Solala, S. A. Losilla, D. Sundholm, W. H. Xu, P. Parkkinen, "Optimization of numerical orbitals using the Helmholtz kernel", J. Chem. Phys. 146 (2017) 084102 DOI: 10.1063/1.4976557.

205. E. Tapavicza, F. Furche, D. Sundholm, "Importance of vibronic effects in the UV-Vis spectrum of the 7,7,8,8-tetracyanoquinodimethane anion", J. Chem. Theory Comput. 12 (2016) 5058-5066 DOI:10.1021/acs.jctc.6b00720.

204. R. Mera-Adasme, W. H. Xu, D. Sundholm, F. Mendizabal, "Calculations of the Light Absorption Spectra of Porphyrinic Chromophores for Dye-Sensitized Solar Cells", Phys. Chem. Chem. Phys. 18 (2016) 27877-27884 DOI:10.1039/C6CP04627D.

203. M. Rauhalahti, A. Muñoz-Castro, D. Sundholm, "Magnetic Response Properties of Gaudiene - A Cavernous and Aromatic Carbocage", Phys. Chem. Chem. Phys. 18 (2016) 18880-18886 DOI: 10.1039/C6CP03808E

202. H. Fliegl, J. Jusélius, D. Sundholm, "Calculations of gauge-origin independent anisotropy of the current density functions", J. Phys. Chem. A 120 (2016) 5658-5664 DOI: 10.1021/acs.jpca.6b03950.

201. D. Sundholm, R. J. F. Berger, H. Fliegl, "Analysis of the Magnetically Induced Current Densities for Molecules Consisting of Annelated Aromatic and Antiaromatic Hydrocarbon Rings", Phys. Chem. Chem. Phys. 18 (2016) 15934-15942 DOI: 10.1039/C6CP01968D.

200. D. Sundholm, H. Fliegl, R. J. F. Berger, "Calculations of Magnetically Induced Current Densities - Theory and Applications", WIREs Comput. Mol. Sci. 6 (2016) 639-678 DOI:10.1002/wcms.1270.

199. C. M. Suomivuori, N. O. Winter, C. Hättig, D. Sundholm, V. R. I. Kaila, "Exploring the Light-Capturing Properties of Photosynthetic Chlorophyll Clusters Using Large-Scale Correlated Calculations", J. Chem. Theory Comput. 12 (2016) 2644-2651. 10.1021/acs.jctc.6b00237.

198. M. Rauhalahti, A. Muñoz-Castro, D. Sundholm, "Thiolate-protected golden fullerenes. A 32-ve core involving a hollow Au_{32} cage", RSC Advances 6 (2016) 21332-21336 DOI: 10.1039/C5RA27683G

197. G. V. Baryshnikov, R. R. Valiev, N. N. Karaush, D. Sundholm, B. F. Minaev, "Aromaticity of the doubly charged [8]circulenes", Phys. Chem. Chem. Phys. 18 (2016) 8980-8992. DOI: 10.1039/C6CP00365F

196. C. M. Suomivuori, L. Lang, D. Sundholm, A. P. Gamiz-Hernandez, V. R. I. Kaila, "Tuning the Protein-Induced Absorption Shifts of Retinal in Engineered Rhodopsin Mimics", Chem. Eur. J. 22 (2016) 8254-8261. DOI:10.1002/chem.201505126.

195. I. Benkyi, H. Fliegl, R. R. Valiev, D. Sundholm, "New Insights on Aromatic Pathways of Carbachlorins and Carbaporphyrins Based on Calculations of Magnetically Induced Current Densities", Phys. Chem. Chem. Phys. 18 (2016) 11932-11941. DOI:10.1039/C5CP06987D

194. H. Fliegl, Z. Q. You, C. P. Hsu, D. Sundholm, "The excitation spectra of naphthalene dimers: Frenkel and charge-transfer excitons", J. Chin. Chem. Soc. 63 (2016) 20-32. DOI:10.1002/jccs.201500368. (Best paper award)

193. R. V. Bojan, J. M. López-de-Luzuriaga, M. Monge, M. E. Olmos, R. Echeverría, O. Lehtonen, D. Sundholm, "Double Jahn-Teller Distortion in Au-Ge Complexes Leading to a Dual Blue-Orange Emission" ChemPlusChem 81 (2016) 176-186. DOI: 10.1002/cplu.201500337

192. D. Du, D. Sundholm, H. Fliegl, "Evaluating Shielding-Based Ring-Current Models by Using the Gauge-Including Magnetically Induced Current Method", J. Chin. Chem. Soc. 63 (2016) 93-100. DOI: 10.1002/jccs.201500027.

191. D. Sundholm, L. N. Wirz, P. Schwerdtfeger, "Novel hollow all-carbon structures", Nanoscale 7 (2015) 15886-15894. DOI: 10.1039/C5NR04370K

190. A. P. Gamiz-Hernandez, R. Send, I. Angelova, D. Sundholm, V. R. I. Kaila, "Protein-Induced Color Shift of Carotenoids in β-Crustacyanin", Angew. Chem. Int. Ed. 54 (2015) 1-4. DOI: 10.1002/anie.201501609.

189. R. R. Valiev, H. Fliegl, D. Sundholm, "Predicting the Degree of Aromaticity of Novel Carbaporphyrinoids", Phys. Chem. Chem. Phys. 17 (2015) 14215-14222. DOI: 10.1039/C5CP01306B.

188. E. A. Toivanen, S. A. Losilla, D. Sundholm, "Grid-based fast multipole method - a massively parallel finite-element scheme for solving the electronic Coulomb problem", Phys. Chem. Chem. Phys. 17 (2015) 31480-31490. DOI:10.1039/C5CP01173F.

187. S. A. Losilla, M. A. Watson, A. Aspuru-Guzik, D. Sundholm, "Construction of the Fock matrix on a grid-based molecular orbital basis using GPGPUs", J. Chem. Theory Comput. 11 (2015) 2053-2062. DOI: 10.1021/ct501128u

186. H. Rabaâ, H. Khaledi, M. M. Olmstead, D. Sundholm, "Computational studies of a paramagnetic planar dibenzotetraaza[14]annulene Ni(II) complex", J. Phys. Chem. A 119 (2015) 5189-5196. DOI: 10.1021/jp509824z

185. R. Send, C. M. Suomivuori, V. R. I. Kaila, D. Sundholm, "Coupled-cluster studies on extended green fluorescent protein models", J. Phys. Chem. B 119 (2015) 2933-2945. DOI: 10.1021/jp5120898.

184. R. R. Valiev, H. Fliegl, D. Sundholm, "Aromatic Pathways of Carbathioporphyrins", J. Phys. Chem. A 119 (2015) 1201-1207. DOI: 10.1021/jp5120652

183. H. Fliegl, F. Pichierri, D. Sundholm, "Antiaromatic Character of 16 π Electron Octaethylporphyrins: Magnetically Induced Ring Currents from DFT-GIMIC Calculations", J. Phys. Chem. A 119 (2015) 2344-2350. DOI: 10.1021/jp5067549

182. R. Mera-Adasme, K. Sadeghian, D. Sundholm, C. Ochsenfeld, "The effect of including torsional parameters for histidine–metal interactions in classical force fields for metalloproteins", J. Phys. Chem. B, 118 (2014) 13106-13111. DOI: 10.1021/jp5078906

181. M. Pohjoispää, R. Mera-Adasme, D. Sundholm, S. Heikkinen, T. Hase, K. Wähälä," Capricious selectivity in electrophilic aromatic deuteration of methylenedioxy substituted compounds", J. Org. Chem. 79 (2014) 10636-10640. DOI: 10.1021/jo5019427.

180. N. Özcan, J. Mareš, D. Sundholm, J. Vaara, Solvation chemical shifts of perylenic antenna molecules from molecular dynamics simulations, Phys. Chem. Chem. Phys. 16 (2014) 22309-22320. DOI: 10.1039/c4cp02894e

179. D. Sundholm "A comment to *Catalyst Induced Hydrino Transition (CIHT) electrochemical cell*", Intern. J. Energy Res. 38 (2014) 1766. DOI: 10.1002/er.3252

178. R. R. Valiev, H. Fliegl, D. Sundholm, "The aromatic character of thienopyrrole-modified 20π-electron porphyrinoids", Phys. Chem. Chem. Phys. 16 (2014) 11010-11016. DOI: 10.1039/C4CP00883A

177. D. Sundholm "On energetic prerequisites of attracting electrons", J. Chem. Phys. 140 (2014) 234111. DOI: 10.1063/1.4883676

176. H. Rabaâ, S. Ghosh, D. Sundholm, J. F. Halet, J. Y. Saillard, "Addition and Elimination Reactions of H_2 in Ruthenaborane Clusters: A Computational Study", J. Organomet. Chem. 761 (2014) 1-9. DOI: 10.1016/j.jorganchem.2014.03.001

175. V. A. Ovchinnikov, D. Sundholm, "Coupled-cluster and density functional theory calculations of the 0–0 bands of the electronic excitation spectra of the DNA bases", Phys. Chem. Chem. Phys. 16 (2014) 6931-6941. DOI: 10.1039/C3CP55080J

174. X. Zhou, D. Sundholm, T. Wesołowski, V. R. I. Kaila, "Spectral Tuning of Rhodopsin and Visual Cone Pigments", J. Am. Chem. Soc. 136 (2014) 2723-2726. DOI: 10.1021/ja411864m

173. H. Fliegl, D. Sundholm, "Coupled-cluster calculations of the lowest 0–0 bands of the electronic excitation spectrum of naphthalene", Phys. Chem. Chem. Phys. 16 (2014) 9859-9865. DOI: 10.1039/C3CP54421D

172. R. V. Bojan, J. M. López-De-Luzuriaga, M. Monge, M. Olmos, R. Echeverría, O. Lehtonen, D. Sundholm "Double Photoinduced Jahn-Teller Distortion of Tetrahedral Au(I)-Sn(II) complexes", ChemPlusChem 79 (2014) 67-76. DOI: 10.1002/cplu.201300314

171. R. Mera-Adasme, C. M. Suomivuori, A. Fierro, J. Pesonen, D. Sundholm, "The role of solvent exclusion in the interaction between D124 and the metal site in SOD1: Implications for ALS", J. Biol. Inorg. Chem. 18 (2013) 931-938. DOI: 10.1007/s00775-013-1039-8

170. R. R. Valiev, H. Fliegl, D. Sundholm, "Insights into magnetically induced current pathways and optical properties of isophlorins", J. Phys. Chem. A 117 (2013), 9062-9068. DOI: 10.1021/jp404828n

169. M. Mehine, S. A. Losilla, D. Sundholm, "An efficient algorithm for calculating three-electron integrals for Gaussian-type orbitals using numerical integration", Mol. Phys. 111 (2013) 2536-2543. DOI: 10.1080/00268976.2013.793847

168. H. Rabaâ, S. Taubert, D. Sundholm, "Computational studies of the electronic absorption spectrum of [(2,2′;6′,2″-terpyridine)-Pt(II)-OH] [7,7,8,8-tetracyanoquinodimethane] complex", J. Phys. Chem. A 117 (2013) 12363-12373. DOI: 10.1021/jp408747d

167. H. Fliegl, N. Özcan, R. Mera-Adasme, F. Pichierri, J. Jusélius, D. Sundholm, "Aromatic pathways in thieno-bridged porphyrins: understanding the influence of the direction of the thiophene ring on the aromatic character", Mol. Phys. 111 (2013) 1364-1372. DOI: 10.1080/00268976.2013.794397

166. D. Sundholm, "C_{72}: Gaudiene a Hollow and Aromatic All-Carbon Molecule", Phys. Chem. Chem. Phys. 15 (2013) 9025-9028. DOI: 10.1039/C3CP51042E

165. M. Touil, N. Hajjaji, D. Sundholm, H. Rabaâ, "Computational studies of the corrosion-inhibition efficiency of iron by triazole surfactants", Intern. J. Quantum Chem. 113 (2013) 1365-1371. DOI: 10.1002/qua.24310

164. V. R. I. Kaila, R. Send, D. Sundholm, "Electrostatic spectral tuning mechanism of the green fluorescent protein", Phys. Chem. Chem. Phys. 15 (2013) 4491-4495. DOI: 10.1039/C3CP00058C

163. R. R. Valiev, E. G. Ermolina, R. T. Kuznetsova, V. N. Cherepanov, D. Sundholm, "Computational and experimental studies of the electronic absorption spectra of EDTA and DTPA substituted tetraphenylporphyrins and their Lu complexes", J. Mol. Model. 19 (2013) 4613-4637. DOI 10.1007/s00894-012-1400-9

162. M. Kaipio, M. Patzschke, H. Fliegl, F. Pichierri, D. Sundholm, "The effect of fluorine substitution on the aromaticity of polycyclic hydrocarbons", J. Phys. Chem. A 116 (2012) 10257-10268. DOI: 10.1021/jp308121b

161. S.A. Losilla, M. Mehine, D. Sundholm, "Construction of the two-electron contribution to the Fock matrix by numerical integration", Mol. Phys. 110 (2012) 2569-2578. DOI: 10.1080/00268976.2012.720725.

160. R. R. Valiev, V. Cherepanov, D. Sundholm, "Computational studies of photophysical properties of porphin, tetraphenylporphyrin and tetrabenzoporhyrin", Phys. Chem. Chem. Phys. 14 (2012) 11508-11517. DOI: 10.1039/C2CP40468K

159. R. Mera-Adasme, F. Mendizábal, M. Gonzalez, S. Miranda-Rojas, C. Olea-Azar, D. Sundholm, "Computational studies of the Metal-binding Site of the Wild-type and the H46R Mutant of the Copper, Zinc Superoxide Dismutase", Inorg. Chem. 51 (2012) 5561-5588. DOI: 10.1021/ic202416d

158. D. Sundholm, T. Vänskä, "Computational Methods for Studies of Semiconductor Quantum Dots and Rings", Annu. Rep. Prog. Chem., Sect. C, 108 (2012) 96-125. DOI: 10.1039/C2PC90004A

157. H. Fliegl, D. Sundholm, "Aromatic pathways of porphins, chlorins and bacteriochlorins", J. Org. Chem. 77 (2012) 3408-3414. DOI: 10.1021/jo300182b

156. M. Pabst, D. Sundholm, A. Köhn, "Ab Initio Studies of Triplet-State Properties for Organic Semiconductor Molecules", J. Phys. Chem. C 116 (2012) 15203-15217. DOI: 10.1021/jp302010a

155. Y.C. Lin, D. Sundholm, "Computational Studies of Non-Stoichiometric Sodium-Auride Clusters", J. Phys. Chem. A 116 (2012) 5119-5128. DOI: 10.1021/jp302124v

154. S.A. Losilla, D. Sundholm, "A divide and conquer real-space approach for calculation of electrostatic potentials and electronic interaction energies for molecules", J. Chem. Phys. 136 (2012) 214104(1-10). DOI: 10.1063/1.4721386

153. V.R.I. Kaila, R. Send, D. Sundholm, "The effect of protein environment on photoexcitation properties of retinal", J. Phys. Chem. B 116 (2012) 2249-2258. DOI: 10.1021/jp205918m

152. M.P. Johansson, V.R.I. Kaila, D. Sundholm, "Ab initio, density functional theory, and semi-empirical calculations", Chapter 1 in "Biomolecular simulations - Methods and Protocols", Eds. E. Salonen and L. Monticelli, Humana Press, Springer, New York, volume 924 in the series "Methods in Molecular Biology" (2012) 3-27, ISBN-10: 1627030166

151. H. Fliegl, D. Sundholm, F. Pichierri, "Aromatic Pathways in Mono- and Bisphosphorous Singly Möbius Twisted [28] and [30]Hexaphyrins", Phys. Chem. Chem. Phys. 13 (2011) 20659-20665. DOI: 10.1039/C1CP21935A

150. H. Fliegl, S. Taubert, O. Lehtonen, D. Sundholm, "The gauge including magnetically induced current method", Phys. Chem. Chem. Phys. 13 (2011) 20500-20518. DOI: 10.1039/C1CP21812C

149. H. Fliegl, O. Lehtonen, M. Patzschke, D. Sundholm, Y.C. Lin, "Theoretical investigation of photoelectron spectra and magnetically induced current densities in ring-shaped transition-metal oxide", Theoret. Chem. Acc. 129 (2011) 701-713. doi:10.1007/s00214-011-0946-4

148. R. Send, V.R.I. Kaila, D. Sundholm, "Reduction of the virtual space for coupled-cluster excitation energies of large molecules and embedded systems", J. Chem. Phys. 134 (2011) 214114:1-9; Virtual J. Biol. Phys. Res., June 15, 2011, doi:10.1063/1.3596729

147. R. Send, V.R.I. Kaila, D. Sundholm, "Benchmarking the coupled-cluster approximate singles and doubles method on biochromophores", J. Chem. Theory Comput. 7 (2011) 2473-2484, doi: 10.1021/ct200215

146. D. Sundholm, "On the superconductor mechanism of [bis(ethylenedithio)tetraselenafulvalene]$_2$GaCl$_4$", Chem. Phys. Letters 503 (2011) 244-246. doi:10.1016/j.cplett.2011.01.037

145. V.R.I. Kaila, E. Oksanen, A. Goldman, M.I. Verkhovsky, D. Sundholm, M. Wikström, "A Combined Quantum Chemical and Crystallographic Study on the Oxidized Binuclear Center of Cytochrome c Oxidase", Biochimica et Biophysica Acta - Bioenergetics 1807 (2011) 769-778. doi:10.1016/j.bbabio.2010.12.016

144. S. Taubert, J. Jusélius, D. Sundholm, "Calculation of spin-current densities using gauge-including atomic orbitals", J. Chem. Phys. 134 (2011) 054123 DOI:10.1063/1.3549567.

143. H. Fliegl, O. Lehtonen, D. Sundholm, V.R.I. Kaila, "Hydrogen-bond strengths by magnetically induced currents", Phys. Chem. Chem. Phys. 13 (2011) 434-437. DOI: 10.1039/C0CP00622J

142. S. Taubert, V.R.I. Kaila, D. Sundholm, "Aromatic pathways in conjugated rings connected by single bonds", Intern. J. Quantum Chem. 111 (2011) 848-857. DOI: 10.1002/qua.22869.

141. T. Vänskä, D. Sundholm, "Interpretation of the photoluminescence spectrum of double quantum rings", Phys. Rev. B 82 (2010) 085306. DOI: 10.1103/PhysRevB.82.085306

140. V.R.I. Kaila, M.P. Johansson, D. Sundholm, M. Wikström, "Inter-heme electron tunneling in cytochrome *c* oxidase", Proc. Natl. Acad. Sci. (USA) 107 (2010) 21470-21475. DOI:10.1073/pnas.1005889107

139. H. Fliegl, D. Sundholm, S. Taubert, F. Pichierri, "The Aromatic Pathways in Twisted Hexaphyrins", J. Phys. Chem. A 114 (2010) 7153-7161. DOI: 10.1021/jp1021517

138. S. Taubert, D. Sundholm, F. Pichierri, "Magnetically Induced Currents in [*n*]Cycloparaphenylenes, *n*=6-11", J. Org. Chem. 75 (2010) 5867-5874. DOI: 10.1021/jo100902w

137. D. Sundholm, S. Taubert, F. Pichierri, " Calculation of absorption and emission spectra of [*n*]cycloparaphenylenes: the reason for the large Stokes shift", Phys. Chem. Chem. Phys. 12 (2010) 2751-2757. DOI: 10.1039/b922175a

136. S.A. Losilla, D. Sundholm, J. Jusélius, "The Direct Approach to Gravitation and Electrostatics Method with Periodic Boundary Conditions", J. Chem. Phys. 132 (2010) 024102. DOI:10.1063/1.3291027

135. H. Fliegl, D. Sundholm, S. Taubert, J. Jusélius, W. Klopper, "Magnetically Induced Current Densities in Aromatic, Antiaromatic, Homoaromatic, and Nonaromatic Hydrocarbons", J. Phys. Chem. A 113 (2009) 8668-8676. DOI: 10.1021/jp9029776

134. O. Lehtonen, D. Sundholm, R. Send, M.P. Johansson, "Coupled-cluster and density functional theory studies of the electronic excitation spectra of *trans*-1,3-butadiene and *trans*-2-propeniminium", J. Chem. Phys. 131 (2009) 024301(1-13). DOI:10.1063/1.3158990

133. S. Taubert, D. Sundholm, F. Pichierri, "Magnetically Induced Currents in Bianthraquinodimethane-Stabilized Möbius and Hückel [16]Annulenes", J. Org. Chem. 74 (2009) 6495-6502. DOI: 10.1021/jo900736d

132. R. Send, D. Sundholm, M.P. Johansson, F. Pawłowski, "Excited-state potential energy surfaces of polyenes and protonated Schiff bases", J. Chem. Theory Comput., 5 (2009) 2401-2414. DOI: 10.1021/ct900240s

131. V.R.I. Kaila, M.P. Johansson, D. Sundholm, L. Laakkonen, M. Wikström, "The Chemistry of the Cu_B Site in Cytochrome c Oxidase and the Importance of its Unique His-Tyr Bond", Biochimica et Biophysica Acta - Bioenergetics 1787 (2009) 221-233.

130. S. Taubert, D. Sundholm, J. Jusélius, H. Fliegl, W. Klopper, "Calculation of magnetically induced currents in hydrocarbon nanorings", J. Phys. Chem. A 112 (2008) 13584-13592.

129. M.P. Johansson, J. Vaara, D. Sundholm, "Exploring the stability of golden fullerenes", J. Phys. Chem. C 112 (2008) 19311-19315. DOI: 10.1021/jp808076f.

128. J. Jusélius, D. Sundholm, "Polycyclic Antiaromatic Hydrocarbons", Phys. Chem. Chem. Phys. 10 (2008) 6630-6634. DOI: 10.1039/b808082h

127. O. Lehtonen, D. Sundholm, T. Vänskä, "Computational studies of semiconductor quantum dots", Phys. Chem. Chem. Phys. 10 (2008) 4535-4550. DOI:10.1039/B804212H

126. S. Taubert, M. Straka, T. Pennanen, D. Sundholm, J. Vaara, "Dynamics, bonding and magnetic resonance properties of $Sc_3C_2@C_{80}$ and its monoanion", Phys. Chem. Chem. Phys. 10 (2008) 7158-7168. DOI: 10.1039/b811032h

125. R. Send, D. Sundholm, "The molecular structure of a curl-shaped retinal isomer", J. Mol. Model. 14 (2008) 717-726.

124. O. Lehtonen, D. Sundholm, "Computational studies of free-standing silicon nanoclusters", Chapter 3 in "Silicon Nanophotonics", Ed. L. Khriachtchev, World Scientific, (2008) ISBN-13 978-981-4241-11-3, pp. 61-88.

123. R. Send, D. Sundholm, "Stairway to the Conical Intersection: A Computational Study of the Retinal Isomerization", J. Phys. Chem. A 111 (2007) 8766-8773.

122. R. Send, D. Sundholm, " Coupled-Cluster Studies of the Lowest Excited States of the 11-*cis*-Retinal Chromophore, Phys. Chem. Chem. Phys. 9 (2007) 2862-2867.

121. L.F. Cui, X. Li, L.S. Wang, Y.C. Lin, D. Sundholm, "Photoelectron Spectroscopic and Computational Studies of Sodium Auride Clusters: $Na_nAu_n^-$ (n=1–3)", J. Phys. Chem. A 111 (2007) 7555-7561.

120. T. Vänskä, M. Lindberg, D. Sundholm, "Configuration-Interaction Studies of Bose-Einstein Condensates", Phys. Rev. A 75 (2007) 023621(1-8).

119. J. Jusélius, D. Sundholm, "Parallel Implementation of a Direct Method for Calculating Electrostatic Potentials", J. Chem. Phys. 126 (2007) 094101 (1-9).

118. R. Send, D. Sundholm, "The Role of the β-Ionone Ring in the Photochemical Reaction of Rhodopsin", J. Phys. Chem. A 111 (2007) 27-33.

117. O. Lehtonen, D. Sundholm, "Optical Properties of Sila-Adamantane Nanoclusters from Density-Functional Theory", Phys. Rev. B 74 (2006) 045433(1-11).

116. O. Lehtonen, D. Sundholm, "Bright Luminescence from Silane Substituted and Bridged Silicon Nanoclusters", Phys. Chem. Chem. Phys. 8 (2006) 4228-4232.

115. O. Lehtonen, D. Sundholm, "Coupled-Cluster Studies of the Electronic Excitation Spectra of Silanes", J. Chem. Phys. 125 (2006) 144314 (1-9).

114. Y.C. Lin, D. Sundholm, J. Jusélius, "On the Aromaticity of the Planar Hydrogen Bonded $(HF)_3$ Trimer", J. Chem. Theory Comput. 2 (2006) 761-764. DOI: 10.1021/ct050297x

113. T. Vänskä, M. Lindberg, J. Olsen, D. Sundholm, "Ab Initio Computational Methods for Studies of Multiexciton Complexes", Phys. Stat. Sol. (b), 243 (2006) 4035-4045.

112. Y.C. Lin, D. Sundholm, J. Jusélius, L.F. Cui, X. Li, H.J. Zhai, L.S. Wang, "Experimental and Computational Studies of Alkali-Metal Coinage-Metal Clusters", J. Phys. Chem. A 110 (2006) 4244-4250.

111. S. Taubert, H. Konschin, D. Sundholm, "Computational Studies of ^{13}C NMR Chemical Shifts for Saccharides", Phys. Chem. Chem. Phys. 7 (2005) 2561-2569.

110. Y.C. Lin, J. Jusélius, D. Sundholm, J. Gauss, "Magnetically Induced Current Densities in Al_4^{2-} and Al_4^{4-} Species Studied at the Coupled-Cluster Level", J. Chem. Phys. 122 (2005) 214308 (1-9). DOI: 10.1063/1.1924590

109. O. Lehtonen, D. Sundholm, "Density-Functional Studies of Excited States of Silicon Nanoclusters" Phys. Rev. B 72 (2005) 085424 (1-8); Virtual J. Nanoscale Sci. & Tech. August 22, 2005.

108. M. Patzschke, D. Sundholm, "Density-Functional-Theory Studies of the Infrared Spectra of Titanium-Carbide Nanocrystals", J. Phys. Chem. B 109 (2005) 12503-12508.

107. M.P. Johansson, J. Jusélius, D. Sundholm, "Sphere Currents of Buckminsterfullerene", Angew. Chem. Int. Ed. 44 (2005) 1843-1846. DOI: 10.1002/anie.200462348

106. R.J.F. Berger, M. Patzschke, H. Schmidbaur, D. Schneider, D. Sundholm, "Isomeric Mono- and Bis[(phosphane)gold(I)] Thiocyanate Complexes", Chem. Eur. J. 11 (2005) 3574-3582.

105. D. Sundholm, "Universal Method for Computation of Electrostatic Potentials", J. Chem. Phys. 122 (2005) 194107 (1-5).

104. R.J.F. Berger, D. Sundholm, "A Non-Iterative Numerical Solver of Poisson and Helmholtz Equations using High-Order Finite-Element Functions", Adv. Quantum Chem. 50 (2005) 235-247. Elsevier ISBN: 0-12-034850-0.

103. K.O.E. Henriksson, K. Nordlund, K. Keinonen, D. Sundholm, M. Patzschke, "Simulations of the Initial Stages of Blistering in Helium Implanted Tungsten", Physica Scripta T108 (2004) 95–98.

102. D. Sundholm, T. Vänskä, "A Full Configuration Interaction Method for Bosonic Systems", J. Phys. B: At. Mol. Opt. Phys. 37 (2004) 2933-2942.

101. Z. Chen, T. Heine, D. Sundholm, P. von Ragué Schleyer, "Aromaticity Indices from Magnetic Shieldings", Chapter 24 in *Quantum Chemical Calculation of Magnetic Resonance Properties*, Eds. M. Kaupp, M. Bühl, V. Malkin, Wiley-VCH, Weinheim ISBN: 3-527-30779-6 (2004) 395-407.

100. J. Jusélius, J. Gauss, D. Sundholm, "Calculation of Current Densities using Gauge-Including Atomic Orbitals" J. Chem. Phys. 121 (2004) 3952-3963. DOI: 10.1063/1.1773136

99. D. Sundholm "Density Functional Studies of the Luminescence of $Si_{29}H_{36}$", Phys. Chem. Chem. Phys 6 (2004) 2044-2047.

98. M.P. Johansson, D. Sundholm, J. Vaara, "Au_{32}: A 24-Carat Golden Fullerene", Angew. Chem. 43 (2004) 2678-2681; Angew. Chem. Int. Ed. 43 (2004) 2678-2681.

97. M.P. Johansson, D. Sundholm, "Spin and Charge Distributions in Iron Porphyrin Models: a Coupled-Cluster and Density-Functional Study", J. Chem. Phys. 120 (2004) 3229-3236.

96. J. Autschbach, B.A. Hess, M.P. Johansson, J. Neugebauer, M. Patzschke, P. Pyykkö, M. Reiher, D. Sundholm, "Properties of WAu_{12}", Phys. Chem. Chem. Phys. 6 (2004) 11-22.

95. D. Sundholm, "A Density-Functional-Theory Study of Bacteriochlorophyll *b*", Phys. Chem. Chem. Phys. 5 (2003) 4265-4271.

94. D. Sundholm, "First Principles Calculations of the Absorption Spectrum of $Si_{29}H_{36}$", Nano Letters 3 (2003) 847-849.

93. S. Corni, M. Braskén, M. Lindberg, J. Olsen, D. Sundholm, "Stabilization Energies of Charged Multiexciton Complexes Calculated at Configuration Interaction Level", Physica E 18 (2003) 436-442.

92. J. Jusélius, M. Patzschke, D. Sundholm, "Calculation of Ring-Current Susceptibilities for Potential Homoaromatic Molecules", J. Mol. Struct. THEOCHEM 633 (2003) 123-136.

91. D. Sundholm, "Perturbation Energy Expansions Based on Two-Component Relativistic Hamiltonians", Theor. Chem. Acc. 110 (2003) 144-152.

90. S. Corni, J. Olsen, M. Braskén, M. Lindberg, D. Sundholm, "Electron-Hole Recombination Density Matrices Obtained from Large Configuration-Interaction Expansions", Phys. Rev. B 67 (2003) 085314.

89. S. Corni, J. Olsen, M. Braskén, M. Lindberg, D. Sundholm, "Size Dependence of the Electron-Hole Recombination Rates in Semiconductor Quantum Dots", Phys. Rev. B 67 (2003) 045313; Virtual J. Nanoscale Sci. & Tech. January 27, 2003.

88. D. Sundholm, "Perturbation Theory Based on Quasi-Relativistic Hamiltonians", Chapter 13 in *Relativistic Electronic Structure Theory, Part 1. Fundamentals*, Ed. P. Schwerdtfeger, Elsevier (2002), ISBN: 0-444-51249-7, 758-792.

87. M.P. Johansson, D. Sundholm, G. Gerfen, M. Wikström, "The Spin Distribution in Low-Spin Iron Porphyrins", J. Am. Chem. Soc. 124 (2002) 11771-11780.

86. M.P. Johansson, M.R.A. Blomberg, D. Sundholm, M. Wikström, "Change in Electron and Spin Density Upon Electron Transfer to Haem *a*", Biochimica et Biophysica Acta - Bioenergetics 1553 (2002) 183-187.

85. M. Braskén, S. Corni, M. Lindberg, J. Olsen, D. Sundholm, "Full Configuration Interaction Studies of Phonon and Photon Transition Rates in Semiconductor Quantum Dots", Mol. Phys. 100 (2002) 911-918.

84. J. Bieroń, P. Pyykkö, D. Sundholm, V. Kellö, A.J. Sadlej, "Nuclear Quadrupole Moments of Bromine and Iodine from Combined Atomic and Molecular Data", Phys. Rev. A 64 (2001) 052507(1-12).

83. J. Jusélius, M. Straka, D. Sundholm, "Magnetic Shielding Calculations on Al_4^{2-} and Analogues. A New Family of Aromatic Molecules?", J. Phys. Chem. A 105 (2001) 9939-9944.

82. R.J.F. Berger, M.A. Schmidt, J. Jusélius, D. Sundholm, H. Schmidbaur, "Tetraberyllium-η^4-oxo-hexa(arylcarboxylates)", Z. Naturforsch. 56 b (2001) 979-989.

81. M. Braskén, M. Lindberg, D. Sundholm, J. Olsen, "Spatial Carrier-Carrier Correlations in Strain-Induced Quantum Dots", Phys. Rev. B 64 (2001) 035312(1-9).

80. J. Jusélius, D. Sundholm, "The Aromaticity and Antiaromaticity of Dehydroannulenes", Phys. Chem. Chem. Phys. 3 (2001) 2433-2437.

79. R.J.F. Berger, M. Hartmann, P. Pyykkö, D. Sundholm, H. Schmidbaur, "The Quest for Beryllium Peroxides", Inorg. Chem. 40 (2001) 2270-2274.

78. M. Braskén, M. Lindberg, D. Sundholm, J. Olsen, "Full Configuration Interaction Calculations of Electron-Hole Correlation Effects in Strain-induced Quantum Dots", Phys. Stat. Sol. (b) 224 (2001) 775-779.

77. M. Braskén, M. Lindberg, D. Sundholm, J. Olsen, "Electron-Hole Correlation Effects in Strain-Induced Quantum Dots", Conference Proceedings Vol. 71 "Atoms, Molecules and Quantum Dots in Laser Fields: Fundamental Processes", Pisa 2000, Edited by N. Bloembergen, N. Rahman, and A. Rizzo, Societa' Italiana di Fisica, Bologna, 2001, pp 315-324.

76. M. Braskén, M. Lindberg, D. Sundholm, J. Olsen, "Carrier-Carrier Correlations in Strain-Induced Quantum Dots", Phys. Stat. Sol. (b) 221 (2000) 37-41.

75. J. Jusélius, D. Sundholm, "The Aromatic Character of Magnesium Porphyrins", J. Org. Chem. 65 (2000) 5233-5237.

74. E.J. Fernández, M.C. Gimeno, A. Laguna, J.M. López-de-Luzuriaga, M. Monge, P. Pyykkö, D. Sundholm, "Luminescent Detection of an Oligomerization Process in Solution through Gold-Gold Interactions. DFT Calculations on $[Au_2Ag_2R_4L_2]_n$ Moieties", J. Am. Chem. Soc. 122 (2000) 7287-7293.

73. D. Sundholm "Interpretation of the Electronic Absorption Spectrum of Free-Base Porphin Using Time-Dependent Density-Functional Theory", Phys. Chem. Chem. Phys. 2 (2000) 2275-2281.

72. J. Jusélius, D. Sundholm, "The Aromatic Pathways of Porphins, Chlorins and Bacteriochlorins", Phys. Chem. Chem. Phys. 2 (2000) 2145-2151.

71. M. Braskén, M. Lindberg, D. Sundholm, J. Olsen, "Full Configuration Interaction Calculations of Electron-Hole Correlation Effects in Strain-Induced Quantum Dots", Phys. Rev. B 61 (2000) 7652-7655.

70. D. Sundholm "Density-Functional-Theory Study of the Electronic Absorption Spectrum of Mg-Porphyrin and Mg-Etioporphyrin-I", Chem. Phys. Letters 317 (2000) 392-399.

69. P.-O. Åstrand, K. Ruud, D. Sundholm, "A Modified Variation-Perturbation Approach to Zero-Point Vibrational Motion", Theor. Chem. Acc. 103 (2000) 365-373.

68. D. Sundholm "Comparison of the Electronic Excitation Spectra of Chlorophyll *a* and Pheophytin *a* Calculated at Density-Functional-Theory Level", Chem. Phys. Letters 317 (2000) 545-552.

67. D. Sundholm, M. Tokman, P. Pyykkö, E. Eliav, U. Kaldor, "Ab Initio Calculations of the Ground-State Electron Affinities of Gallium and Indium", J. Phys. B: At. Mol. Opt. Phys 32 (1999) 5853-5859.

66. J. Jusélius, D. Sundholm "Ab Initio Determination of the Induced Ring Current in Aromatic Molecules", Phys. Chem. Chem. Phys. 1 (1999) 3429-3435.

65. V. Kellö, A.J. Sadlej, P. Pyykkö, D. Sundholm, M. Tokman, "Electric Quadrupole Moment of the ^{27}Al Nucleus: Converging Results from the AlF and AlCl Molecules and the Al Atom", Chem. Phys. Letters 304 (1999) 414-422.

64. D. Sundholm, "Density Functional Theory Calculations of the Visible Spectrum of Chlorophyll *a*", Chem. Phys. Letters 302 (1999) 480-484.
DOI:10.1016/S0009-2614(99)00194-3

63. D. Sundholm, "Finite-Element Multiconfiguration Hartree-Fock Calculations of the Atomic Quadrupole Moment of $Ar^+(^2P_{3/2})$", Phys. Rev. A 59 (1999) 3355-3358.

62. D. Sundholm, H. Konschin, M. Häser, "An Ab Initio Study of the Structure and Energetics of Free-Base Bonellin-Dimethylester Isomers and Transition States", Chem. Eur. J. 5 (1999) 267-273.

61. D. Sundholm, M.R. Sundberg, R. Uggla, "Intermolecular Interactions in *Para*-Chlorobenzoic Acid Dimers", J. Phys. Chem. A 102 (1998) 7137-7142.

60. M. Tokman, D. Sundholm, P. Pyykkö, "Nuclear Quadrupole Moments of Gallium Isotopes Obtained from Finite-Element MCHF Calculations on the $4p\ ^2P_{3/2}$ State of Ga", Chem. Phys. Letters 291 (1998) 414-418.

59. J. Olsen, D. Sundholm, "On Perturbation Expansions of the Extended Koopmans' Theorem", Chem. Phys. Letters 288 (1998) 282-288.

58. K. Nordlund, D. Sundholm, N. Runeberg, "Repulsive Interatomic Potentials Calculated Using Hartree-Fock and Density-Functional Theory Methods", Nucl. Instr. and Meth. in Phys. Res. B 132 (1997) 45-54.

57. D. Sundholm, J. Gauss, "Isotope and Temperature Effects on the Nuclear Magnetic Shielding Tensors and Spin-Rotation Constants Calculated at the Coupled-Cluster Level", Mol. Phys. 92 (1997) 1007-1014.

56. L.L. Lohr, D. Sundholm, "An Ab Initio Characterization of Diphosphorous Trisulfide, P_2S_3", J. Mol. Struct. 413-414 (1997) 495-500.

55. D. Sundholm, E. Ottschofski, "Relativistic Multiconfiguration Hartree-Fock by Means of Direct Perturbation Theory", Intern. J. Quantum Chem. 65 (1997) 151-158.

54. A. Halkier, O. Christiansen, D. Sundholm, P. Pyykkö, "An Improved Value for the Nuclear Quadrupole Moment of the 197 keV $I = \frac{5}{2}$ Excited State of ^{19}F", Chem. Phys. Letters 271 (1997) 273-279.

53. J. Gauss, D. Sundholm, "Coupled Cluster Calculations of Spin-Rotation Constants", Mol. Phys. 91 (1997) 449-458.

52. M. Tokman, D. Sundholm, P. Pyykkö, J. Olsen, "The Nuclear Quadrupole Moment of ^{14}N Obtained from Finite-Element MCHF Calculations on N^{2+} ($2p$; $^2P_{3/2}$) and N^+ ($2p^2$; $^3P_2$ and $2p^2$; $^1D_2$)", Chem. Phys. Letters 265 (1997) 60-64.

51. J. Kobus, L. Laaksonen, D. Sundholm, "A Numerical Hartree-Fock Program for Diatomic Molecules", Computer Phys. Commun. 98 (1996) 346-358; http://laaksonen.csc.fi/num2d.html

50. D. Sundholm, J. Gauss, A. Schäfer, "Rovibrationally Averaged Nuclear Magnetic Shielding Tensors Calculated at the Coupled-Cluster Level", J. Chem. Phys. 105 (1996) 11051-11059.

49. D. Sundholm, "Ab Initio Study of Nuclear Magnetic Shieldings and Ultraviolet Spectra for Hypothiocyanite and its Isomers. The Molecular Structure of Hypothiocyanite", J. Am. Chem. Soc. 117 (1995) 11523-11528.

48. D. Sundholm, J. Gauss, R. Ahlrichs, "The Electron Correlation Contribution to the Nuclear Magnetic Shielding Tensor of the Hydrogen Molecule", Chem. Phys. Letters 243 (1995) 264-268.

47. D. Sundholm, "Core-Valence Correlation Effects on the Ground-State Electron Affinity of Strontium and Barium", J. Phys. B: At. Mol. Opt. Phys. 28 (1995) L399-L404.

46. D. Sundholm, "Numerical Multiconfigurational Hartree-Fock Calculations of Spin and Charge Densities Using the Hiller-Sucher-Feinberg Operator Identity", J. Chem. Phys. 102 (1995) 4895-4903.

45. D. Sundholm, J. Olsen, "Finite-Element Multiconfiguration Hartree-Fock Calculations of Electron Affinities of Manganese", Chem. Phys. Letters 233 (1995) 115-122.

44. D. Sundholm, P. Jørgensen, J. Olsen, "A Multiconfiguration Self-Consistent-Field Response Study of One- and Two-Photon Dipole Transitions between the $X^1\Sigma^+$ and $A^1\Pi$ States of CO", J. Chem. Phys. 102 (1995) 4143-4150.

43. D. Sundholm, J. Olsen, "Finite-Element Multiconfiguration Hartree-Fock Calculations of the Atomic Quadrupole Moments of $C^+(^2P)$ and $Ne^+(^2P)$", Phys. Rev. A 49 (1994) 3453-56.

42. D. Sundholm, A. Rizzo, P. Jørgensen, "Multiconfiguration Self-Consistent-Field Quadratic Response Calculations of the Two-Photon Transition Probability Rate Constants for Argon", J. Chem. Phys. 101 (1994) 4931-35.

41. D. Sundholm, "Fully Numerical Solutions of Molecular Dirac Equations for Highly Charged One-Electron Homonuclear Diatomic Molecules", Chem. Phys. Letters 223 (1994) 469-473.

40. J. Olsen, L.G.M. Pettersson, D. Sundholm, "Calculations of Excitation Energies and Electron Affinities for Be", J. Phys. B: At. Mol. Opt. Phys. 27 (1994) 5575-86.

39. J. Olsen, D. Sundholm, "The Nuclear Quadrupole Moment of ^{14}N Obtained from Finite Element MCHF Calculations on $N^+(2p3p)\ ^1P$", Chem. Phys. Letters, 226 (1994) 17-21.

38. D. Sundholm, J. Olsen, "Core-Valence Correlation Effects on the Ground-State Electron Affinity of Calcium", Chem. Phys. Letters 217 (1994) 451-455.

37. D. Sundholm, J. Olsen, M. Godefroid, G. Van Meulebeke, "Core-Valence Correlation on the Low-Lying $^{1,3}F^o$ Terms of Ca I", Phys. Rev. A 48 (1993) 3606-3610.

36. D. Sundholm, J. Olsen, "Response to "Comment on 'The Exactness of the Extended Koopmans' Theorem: A Numerical Study' " ", J. Chem. Phys. 99 (1993) 6222-6223.

35. D. Sundholm, J. Olsen, "Finite Element Multiconfiguration Hartree-Fock Calculations of the Atomic Quadrupole Moments of Excited States of Be, Al, In, Ne, Ar, Kr, and Xe", Phys. Rev. A 47 (1993) 2672-2679.

34. D. Sundholm, J. Olsen, "Finite Element Multiconfiguration Hartree-Fock Determination of the Nuclear Quadrupole Moments of Chlorine, Potassium, and Calcium Isotopes", J. Chem. Phys. 98 (1993) 7152-7158.

33. D. Sundholm, J. Olsen, "The Exactness of the Extended Koopmans' Theorem: A Numerical Study", J. Chem. Phys. 98 (1993) 3999-4002.

32. D. Sundholm, J. Olsen, "Finite Element Multiconfiguration Hartree-Fock Determination of the Atomic Quadrupole Moment of Ca(3d4s;^{1}D)", Chem. Phys. Letters 198 (1992) 526-530.

31. D. Sundholm, J. Olsen, "Atomic Determination of the ^{23}Na, ^{25}Mg, and ^{27}Al Nuclear Quadrupole Moments: How Accurate are the Muonic Values?", Phys. Rev. Letters 68 (1992) 927-930.

30. D. Sundholm, J. Olsen, S.A. Alexander, "Finite-Element MCHF Calculations on the Excitation Energies and the Ionization Potential of Oxygen", J. Chem. Phys. 96 (1992) 5229-5232.

29. D. Sundholm, J. Olsen, "Finite-Element Multiconfiguration Hartree-Fock Calculations on Carbon, Oxygen and Neon: The Nuclear Quadrupole Moments of ^{11}C, ^{17}O, and ^{21}Ne", J. Phys. Chem. 96 (1992) 627-630.

28. D. Sundholm, J. Olsen, "Finite Element MCHF Calculations on Excitation Energies and the Ionization Potential of Carbon", Chem. Phys. Letters 182 (1991) 497-502.

27. D. Sundholm, J. Olsen, "Finite Element MCHF Calculations on Mg(3s3p;$^3P^o$): the Nuclear Quadrupole Moment of ^{25}Mg", Nucl. Phys. A 534 (1991) 360-366.

26. D. Sundholm, J. Olsen, "Large MCHF Calculations on the Hyperfine Structure of B(^{2}P) and the Nuclear Quadrupole Moments of ^{10}B and ^{11}B", J. Chem. Phys. 94 (1991) 5051-5055.

25. D. Sundholm, J. Olsen, "Large MCHF Calculations on the Hyperfine Structure of Be($^3P^o$) and the Nuclear Quadrupole Moment of ^{9}Be", Chem. Phys. Letters 177 (1991) 91-97.

24. A.M. Mårtensson-Pendrill, S.A. Alexander, L. Adamowicz, N. Oliphant, J. Olsen, P. Öster, H.M. Quiney, S. Salomonsson, D. Sundholm, "Beryllium Atom Reinvestigated: A Comparison between Theory and Experiment", Phys. Rev. A 43 (1991) 3355-3364.

23. D. Sundholm, J. Olsen, "A Comparison Between Finite-Difference, Finite-Element, and Algebraic Multiconfiguration Hartree-Fock Approaches for Atomic and Molecular Calculations", Proc. 13th IMACS World Congress on Computation and Applied Mathematics, Dublin 1991, Edited by R. Vichnevetsky and J.J.H. Miller, Criterion Press, Dublin (1991), pp 861-862.

22. P. Pyykkö, D. Sundholm, L. Laaksonen, J. Olsen, "Two Fully Numerical Methods in Quantum Chemistry", in "The CP90 Europhysics Conference on Computational Physics", Edited by A. Tenner, World Scientific, Singapore (1991), pp. 455-457.

21. D. Sundholm, J. Olsen, "Large MCHF Calculations on the Electron Affinity of Boron", Chem. Phys. Letters 171 (1990) 53-57.

20. D. Sundholm, J. Olsen, "The Nuclear Quadrupole Moment of ^{33}S and ^{35}S", Phys. Rev. A 42 (1990) 1160-1164.

19. D. Sundholm, J. Olsen, "Large MCHF Calculations on the Hyperfine Structure of Li(^{2}S) and Li(^{2}P)", Phys. Rev. A 42 (1990) 2614-2621.

18. D. Sundholm, J. Olsen, P.Å. Malmqvist, B.O. Roos, "Numerical MCSCF in One and Two Dimensions", in "Numerical Determination of the Electronic Structure of Atoms, Diatomic and Polyatomic Molecules", Proc. NATO Advanced Research Workshop, Versailles 1988, Edited by M. Defranceschi and J. Delhalle. Dordrecht: Reidel, (1989), pp. 329-334.

17. D. Sundholm, "Two-Dimensional Fully Numerical Solution of Molecular Dirac Equations: Dirac-Slater Calculations on LiH, Li_2, BH, and CH^+", Chem. Phys. Letters 149 (1988) 251-256.

16. D. Sundholm, "A Block Preconditioned Conjugate Gradient Method for Solving High-order Finite Element Matrix Equations", Computer Phys. Commun. 49 (1988) 409-415.

15. G.H.F. Diercksen, A.J. Sadlej, D. Sundholm, P. Pyykkö, "Towards an Accurate Determination of the Nuclear Quadrupole Moment of Li from Molecular Data: LiF", Chem. Phys. Letters 143 (1988) 163-168.

14. P. Pyykkö, D. Sundholm, L. Laaksonen, "Two-Dimensional Fully Numerical Molecular Calculations. XI. Hartree-Fock Results for BeH^+, $LiHe^+$, CH^+, NeH^+, C_2, BeO, LiF, NaH, MgH^+, HeNe, LiNa, and F_2", Mol. Phys. 60 (1987) 597-604.

13. D. Sundholm, P. Pyykkö, L. Laaksonen, "Two-Dimensional Fully Numerical Solutions of Second-order Dirac Equations for Diatomic Molecules, Part 3", Physica Scripta 36 (1987) 400-402.

12. L. Laaksonen, P. Pyykkö, D. Sundholm, "Fully Numerical Hartree-Fock Methods for Molecules", Comp. Phys. Reports 4 (1986) 313-344.

11. D. Sundholm, P. Pyykkö, L. Laaksonen, A.J. Sadlej, "Nuclear Quadrupole Moment of Nitrogen from Combined Fully Numerical and Discrete Basis Set Calculations on NO^+ and N_2", Chem. Phys. 101 (1986) 219-225.

10. D. Sundholm, P. Pyykkö, L. Laaksonen, "Two-Dimensional Fully Numerical Molecular Calculations. X. Hartree-Fock Results for He_2, Li_2, Be_2, HF, OH^-, N_2, CO, BF, NO^+, and CN^-", Mol. Phys. 56 (1985) 1411-1418.

9. E.J. Baerends, P. Vernooijs, A. Rozendaal, P.M. Boerrigter, M. Krijn, D. Feil, D. Sundholm, "Basis Set Effects on the Electron Density and Spectroscopic Properties of CO", J. Mol. Struct. THEOCHEM 133 (1985) 147-159.

8. D. Sundholm, P. Pyykkö, L. Laaksonen, "Two-Dimensional Fully Numerical Molecular Calculations. VIII. Electric Field Gradients of Diatomic Hydrides LiH - ClH at the HFS Level", Mol. Phys. 55 (1985) 627-635.

7. D. Sundholm, P. Pyykkö, L. Laaksonen, "Fully Numerical HFS Calculations on Cr_2: Basis Set Truncation Error on the Bond Length and Interaction of the Semicore Orbitals", Finn. Chem. Letters 1985 (1985) 51-55.

6. L. Laaksonen, D. Sundholm, P. Pyykkö, "Two-Dimensional Fully Numerical Molecular Calculations. IV. Hartree-Fock-Slater Results on Second-Row Diatomic Molecules", Intern. J. Quantum Chem. 27 (1985) 601-612.

5. D. Sundholm, P. Pyykkö, L. Laaksonen, A.J. Sadlej, "Nuclear Quadrupole Moment of Lithium from Combined Fully Numerical and Discrete Basis Set Calculations on LiH", Chem. Phys. Letters 112 (1984) 1-9.

4. L. Laaksonen, D. Sundholm, P. Pyykkö, "Two-Dimensional Fully Numerical MCSCF Calculations on H_2 and LiH: The Dipole Moment of LiH", Chem. Phys. Letters 105 (1984) 573-575.

3. L. Laaksonen, P. Pyykkö, D. Sundholm, "Two-Dimensional Fully Numerical Solutions of Molecular Hartree-Fock Equations: LiH and BH", Chem. Phys. Letters 96 (1983) 1-3.

2. L. Laaksonen, P. Pyykkö, D. Sundholm, "Two-Dimensional Fully Numerical Solutions of Molecular Schrödinger Equations. II. Solutions of the Poisson Equation and Results for Singlet States of H_2 and HeH^+", Intern. J. Quantum Chem. 23 (1983) 319-323.

1. L. Laaksonen, P. Pyykkö, D. Sundholm, "Two-Dimensional Fully Numerical Solutions of Molecular Schrödinger Equations. I. One-Electron Molecules", Intern. J. Quantum Chem. 23 (1983) 309-317.

B: Non-refereed scientific articles

17. L. Frediani, D. Sundholm, "Editorial; Real-Space Numerical Grid Methods in Quantum Chemistry" Phys. Chem. Chem. Phys. 17 (2015) 31357-31359. DOI 10.1039/c5cp90198g

16. In S. K. Ritter, "Aromaticity For All", Chem. Eng. News **93** (2015) 37-38, contribution to the discussion by D. Sundholm in "Aromaticity By Any Other Name", http://cen.acs.org/articles/93/i8/Aromaticity1.html.

15. S. Riedel, P. Schwerdtfeger, D. Sundholm, "Editorial; The Pekka Pyykkö issue", Theor. Chem. Acc. 129 (2011) 271-289.
DOI 10.1007/s00214-011-0948-2

14. D. Sundholm, R. Send, "Ab initio and density functional theory studies of the retinal isomerization reaction mechanism", CSC Report on Computational Science in Finland 2006-2007, Eds. A. Sillanpää, J. Fagerholm, S. Kotila, J. Ahokas, P. L. Forsström, E. Järvinen, A. M. Sarén, J. Tarus, and E. Vitie, (2007) 76-78. ISBN 978-9525520-27-9.

13. M. Johansson, D. Sundholm, "On the Electronic Structure of Haem", CSC Report on Scientific Computing 2001-2003, Eds. S. Kotila, J. Haataja, P. L. Forsström, J. Ignatius, L. Jukka, M. M. Laine, N. Runeberg, P. Råback, V. Savolainen, (2003) 85-88.

12. D.Sundholm, "Nakanishi, K., Berova N., and Woody, R.W., Circular Dichroism: Principles and Applications, VCH Publishers Inc. New York 1994. 570 s. ISBN 1-56081-618-X." Kemia-Kemi 23 (1996) 507.

11. D. Sundholm, "Kahn, O., Molecular Magnetism, VCH Publishers Inc., New York 1993. 380 s. ISBN 1-56081-566-3." Kemia-Kemi 23 (1996) 387.

10. D. Sundholm, P. Pyykkö, "Very Accurate Atomic Structure Calculations", CSC/News, 3 (1991) 1.

9. M. Ekholm, H. Konschin, P. Pyykkö, D. Sundholm, "7th International Congress on Quantum Chemistry", Kemia-Kemi 18 (1991) 848-849.

8. H. Konschin, D. Sundholm, "Kvantkemi, Kvantumbiologi och Kvantumfarmakologi, 31st Sanibel Symposia", Kemia-Kemi 18 (1991) 559-560.

7. D. Sundholm, "Bader R.F.W., Atoms in Molecules, Oxford University Press, Avon GB 1990. 438 s. ISBN 0-19-855168-1", Kemia-Kemi 18 (1991) 6.

6. D. Sundholm, "8th Seminar on Computational Methods in Quantum Chemistry", Kemia-Kemi 17 (1990) 871.

5. D. Sundholm, "10th Canadian Symposium on Theoretical Chemistry", Kemia-Kemi 16 (1989) 1170.

4. L. Laaksonen, D. Sundholm, P. Pyykkö, "Fully Numerical Hartree-Fock Methods for Molecules", in "Scientific Computing in Finland", Eds. K. Kankaala and R. Nieminen, Research Report R1/89, Centre for Scientific Computing, (1989), pp. 183-213.

3. M. Hotokka, D. Sundholm, "Ab Initio Potential Energy Curves for the CH_3F^- and CH_3Cl^- Anions", Finn. Chem. Letters 1985 (1985) 165-165. (abstract)

2. D. Sundholm, "Sanibel Symposia 1984", Kemia-Kemi 11 (1984) 416.

1. K. Kinnari, L. E. Lindfors, D. Sundholm, "Mechanism and Kinetics of Carbon Monoxide Oxidation over Nickel Oxide", Meddelanden från Institutionen för Teknisk Kemi, Åbo Akademi, 1982, 1-21.

C: Scientific book chapters

4. M. Braskén, M. Lindberg, D. Sundholm, J. Olsen, "Electron-Hole Correlation Effects in Strain-Induced Quantum Dots", Conference Proceedings Vol. 71 "Atoms, Molecules and Quantum Dots in Laser Fields: Fundamental Processes", Pisa 2000, Edited by N. Bloembergen, N. Rahman, and A. Rizzo, Societa' Italiana di Fisica, Bologna, 2001, pp 315-324.

3. D. Sundholm, J. Olsen, "A Comparison Between Finite-Difference, Finite-Element, and Algebraic Multiconfiguration Hartree-Fock Approaches for Atomic and Molecular Calculations", Proc. 13th IMACS World Congress on Computation and Applied Mathematics, Dublin 1991, Edited by R. Vichnevetsky and J.J.H. Miller, Criterion Press, Dublin (1991), pp 861-862.

2. P. Pyykkö, D. Sundholm, L. Laaksonen, J. Olsen, "Two Fully Numerical Methods in Quantum Chemistry", in "The CP90 Europhysics Conference on Computational Physics", Edited by A. Tenner, World Scientific, Singapore (1991), pp. 455-457.

1. D. Sundholm, J. Olsen, P.Å. Malmqvist, B.O. Roos, "Numerical MCSCF in One and Two Dimensions", in "Numerical Determination of the Electronic Structure of Atoms, Diatomic and Polyatomic Molecules", Proc. NATO Advanced Research Workshop, Versailles 1988, Edited by M. Defranceschi and J. Delhalle. Dordrecht: Reidel, (1989), pp. 329-334.

E: Publications intended for the general public

16. D. Sundholm, "Numerical Electronic Structure Methods: A Long-term Research Project Funded by the Academy of Finland", Kemiauutiset, University of Helsinki, (2019), 44-45.

15. D. Sundholm, M. P. Johansson, "Winter School in Theoretical Chemistry 2018 - Machine Learning, Kemiauutiset, University of Helsinki, (2019), 34-35.

14. Dage Sundholm "Winter School in Theoretical Chemistry 2015 Computational Biochemistry", Kemiauutiset, University of Helsinki, (2016), 70-71.

13. Dage Sundholm "Sabbatical leave: A great opportunity" Kemiauutiset, University of Helsinki, (2016), 38-39.

12. D. Sundholm "Theoretical f-Element Chemistry The 30th Winter School in Theoretical Chemistry", Kemiauutiset, University of Helsinki, (2015) 73.

11. D. Sundholm "Magnetically Induced Currents in Molecules (MAGIC 2014), Kemiauutiset, University of Helsinki, (2015) 72.

10. D. Sundholm "Winter School Tales", Kemiauutiset, University of Helsinki, (2013) 38.

9. D. Sundholm, "Behövs experiment för att verifiera beräkningar?", Sphinx (2011-12), Societas Scientiarum Fennica, (2012) 93-100

8. D. Sundholm, P. Pyykkö "Professor Björn O. Roos (28.6.1937-22.2.2010) Sveriges ledande beräkningskemist", Hufvustadsbladet, 29.3.2010; Kemia/Kemi 3/2010 p. 52.

7. M. Johansson, D. Sundholm, "Kultaa Palleroina", Tietoyhteys No 1 (2005) 16-18.

6. D. Sundholm, M. Heinrichs, "Meikovandringen", Best 1 (2003) 5.

5. In S. K. Ritter, "Deciphering Metal Aromaticity", Chem. Eng. News **81** (2003) 23-26, contribution to the discussion by D. Sundholm.

4. D. Sundholm "TekNatur 2002", Kirkkonummen Sanomat, 1.12 (2002) 18.

3. H. Konschin, N. Runeberg, D. Sundholm, J. Vaara, "Tarkkoja työkaluja monitieteelliseen tutkimukseen. Kansainvälinen kvanttikemian konferenssi Kuusamossa", Kemia-Kemi 29 (2002) 52.

2. D. Sundholm "En kommentar till Miten mitata luovuutta?", Yliopisto (Acta Universitatis Helsingiensis) 19 (1998) 31-32.

1. D. Sundholm, "Programvara för Molekylmodellering", Meddelanden från Tekniska Läroverket i Helsingfors, Serie B: 1 (1991) 54-63.

G: Thesis

3. D. Sundholm, "Applications of Fully Numerical Two-Dimensional Self-Consistent Methods on Diatomic Molecules", Doctor of Philosophy Thesis, Department of Chemistry, University of Helsinki, Finland (1985), 54+81 pages.

2. D. Sundholm,"Tvådimensionella Numeriska Lösningar till Molekylära Hartree-Fock och Hartree-Fock-Slater Ekvationer", Licentiate of Technology Thesis, Department of Physical Chemistry, Åbo Akademi, Finland, (1983) 27+27 pages.

1. D. Sundholm, "Undersökning av ett Katalytiskt System: Oxidation av Kolmonoxid över Nickeloxid Katalysatorer", Master of Science (Engineering) Thesis, Department of Chemical Engineering, Åbo Akademi, 1981, 73+34 pages.

H: Patents

1. D. Sundholm, "Method and apparatus for computation of electrostatic potential", (2006) patent number US 20060085149 A1.

I: ICT software

12. DAGE: a new efficient approach to compute the electrostatic potentials and electronic structure of molecules; authors: D. Sundholm and J. Jusélius, S. A. Losilla, P. Parkkinen, E. A. Toivanen, W. H. Xu, E. Solala, L. N. Wirz [101,115].

11. 3D-POISSON: a finite-element program for solution of the Poisson equation in three dimensions (3D); authors: R.J.F. Berger and D. Sundholm [100].

10. BOSSE: a direct configuration-interaction program for studies of bosonic systems; authors: D. Sundholm and T. Vänskä [98,116].

9. GIMIC: a novel method to compute magnetically induced current densities in molecular systems; authors: J. Jusélius, D. Sundholm, and J. Gauss [97].

8. 1D-DIRAC: a finite-element program for solution of the Dirac equation and related quasi-relativistic equations for one-electron atoms; author: D. Sundholm [84].

7. QDOT: an *ab initio* configuration-interaction and coupled-cluster program package for studies of the electron-hole interactions in semiconductor quantum dots; authors: M. Braskén, S. Corni, M. Lindberg, D. Sundholm, J. Olsen [81,109].

6. ROVIB: a finite-element program for calculation of rovibrational energies and vibrational transition properties of diatomic molecules; author: D. Sundholm [47]. GNU General Public License, available at http://www.chem.helsinki.fi/∼sundholm/software/GPL/.

5. LUCAS: a finite-element multiconfiguration Hartree-Fock program for studies of the electronic structure of atomic systems; authors: J. Olsen and D. Sundholm [18,23].

4. SCANDIC: a finite-element multiconfiguration Hartree-fock program for studies of the electronic structure of diatomic molecules; authors: D. Sundholm, J. Olsen, and P.-Å. Malmqvist [1 (in conference books)].

3. 2DDFT: a finite-difference density-functional theory program for studies of diatomic molecules; authors: T. Grabo, D. Sundholm, L. Laaksonen, P. Pyykkö [12].

2. 2D-POISSON: a finite-element program for solution of the Poisson equation for diatomic molecular systems; author: D. Sundholm [16].

1. 2DHF: a finite-difference Hartree-Fock program for studies of diatomic molecules; authors: J. Kobus, L. Laaksonen, D. Sundholm and P. Pyykkö [12,48].