

CMS Papers 2009

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Preface

The present report will contain a cumulative record of papers, published by the Finnish Centre of Excellence in Computational Molecular Science ('CMS'). During the fourth year of operation (2009), all papers of the participant groups are included.

Lauri Halonen
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Bibliography

- [1] Järvi T.T., Pohl D., Albe K., Rellinghaus B., Schultz L., Fassbender J., Kuronen A. and Nordlund K. (2009). From multiply twinned to fcc nanoparticles via irradiation-induced transient amorphization. *Eur. Phys. Lett.*, **85**, 26001.
- [2] Pakarinen J.A., Backman M., Djurabekova F. and Nordlund K. (2009). Partial melting mechanisms of embedded nanocrystals. *Phys. Rev. B*, **79**, 085426.
- [3] Djurabekova F., Backman M., Pakarinen O.H., Nordlund K., Araujo L. and Ridgway M. (2009). Amorphization of Ge nanocrystals embedded in amorphous silica under ion irradiation. *Nucl. Instr. Meth. Phys. Res. B*, **267**, 1235–1238.
- [4] Nordlund K. and Samela J. (2009). Atomic flows, coronas and cratering in Au, Si and SiO₂. *Nucl. Instr. Meth. Phys. Res. B*, **267**, 1420–1423.
- [5] Pakarinen O.H., Djurabekova F., Nordlund K., Kluth P. and Ridgway M. (2009). Molecular dynamics simulations of the structure of latent tracks in quartz and amorphous SiO₂. *Nucl. Instr. Meth. Phys. Res. B*, **267**, 1456–1459.
- [6] Airila M., Ikonen T., Borodin D., Kirschner A., Nordlund K. and Loarte A. (2009). Improvement of surface processes modelling in the ERO code. *J. Nucl. Mater*, **390-391**, 175–178.
- [7] Meinander K. and Nordlund K. (2009). Irradiation induced densification of cluster-assembled thin films. *Phys. Rev. B*, **79**, 045411.
- [8] Tymiak N., Chrobak D., Nagao S., Nordlund K., Räisänen J., Gerberich W. and Nowak R. (2009). Comment on "Nanoindentation hardness anisotropy of alumina crystal: A molecular dynamics study" [Appl. Phys. Lett., 92, 161904 2008]. *Appl. Phys. Lett.*, **94**, 146101.
- [9] Henriksson K.O.E. and Nordlund K. (2009). Simulations of cementite: An analytical potential for the Fe-C system. *Phys. Rev. B*, **79**, 144107.
- [10] Terentyev D., Juslin N., Nordlund K. and Sandberg N. (2009). Fast three dimensional migration of He clusters in bcc Fe and Fe-Cr alloys. *J. Appl. Phys.*, **105**, 103509.
- [11] Dudarev S., Boutard J.L., Lässer R., Caturla M., Derlet P., Fivel M., Fu C.C., Lavrentiev M., Malerba L., Mrovec M., Nguyen-Manh D., Nordlund K., Perlado M., Schäublin R., Swygenhoven H.V., Terentyev D., Wallenius J., Weygand D. and Willaime F. (2009). The EU programme for modelling radiation effects in fusion reactor materials: An overview of recent advances and future goals. *J. Nucl. Mater.*, **386-388**, 1–7.
- [12] Vuckovic S., Samela J., Nordlund K. and Popok V.N. (2009). Pinning of size-selected Co clusters on highly ordered pyrolytic graphite. *Eur. Phys. J. D*, **52**, 107–110.
- [13] Björkas C. and Nordlund K. (2009). Assessment of the relation between ion beam mixing, electron-phonon coupling, and damage production in Fe. *Nucl. Instr. Meth. Phys. Res. B*, **267**, 1830–1836.
- [14] Meinander K. and Nordlund K. (2009). Modeling of film growth by cluster deposition: The effect of size and energy. *Phys. Rev. B*, **79**, 235435.

- [15] Popok V.N., Vuckovic S., Campbell E.E.B., J. Jensen J.S. and Nordlund K. (2009). Energetic Cluster-Surface Interactions. *Proceedings of the 2009 Ion-Solid Interactions conference*, **1**, 49.
- [16] Djurabekova F., Backman M., Pakarinen O.H., Nordlund K., Araujo L.L. and Ridgway M.C. (2009). Energetic ion modification of semiconductor nanocrystals embedded in silica: simulation and experiments. *Proceedings of the 2009 Ion-Solid Interactions conference*, **2**, 149.
- [17] Nordlund K., Vörtler K. and Björkas C. (2009). Atomistic simulations of plasma-wall interactions on the first wall of fusion reactors. *Proceedings of the 2009 Ion-Solid Interactions conference*, **?**, ??
- [18] Björkas C., Juslin N., Timko H., Vörtler K., Nordlund K., Henriksson K.O.E. and Erhart P. (2009). Interatomic potentials for the beryllium Be-C-H system. *J. Phys.: Condens. Matter*, **21**, 445002.
- [19] Albe K., Nord J. and Nordlund K. (2009). Dynamic charge-transfer bond-order potential for gallium nitride. *Phil. Mag.*, **89**, 3477–3497.
- [20] Järvi T.T., Kuronen A., Nordlund K. and Albe K. (2009). Low energy cluster deposition of nanoalloys. *J. Appl. Phys.*, **106**, 063516.
- [21] Juslin N. and Nordlund K. (2009). Molecular dynamics simulations of collision cascades in FeCrHe. *Nucl. Instr. Meth. Phys. Res. B*, **267**, 3420–3423.
- [22] Backman M., Djurabekova F., Pakarinen O.H., Nordlund K., Araujo L.L. and Ridgway M.C. (2009). Amorphization of Ge and Si nanocrystals embedded in amorphous SiO₂ by ion irradiation. *Phys. Rev. B*, **80**, 144109.
- [23] Popok V.N., Vuckovic S., Samela J., Järvi T.T., Nordlund K. and Campbell E.E.B. (2009). Stopping of energetic cobalt clusters and formation of radiation damage in graphite. *Phys. Rev. B*, **80**, 205419.
- [24] Björkas C., Vörtler K., Nordlund K., Nishijima D. and Doerner R. (2009). Chemical sputtering of Be due to D bombardment. *New J. Phys.*, **11**, 123017.
- [25] Henriksson K. (2009). Helium atoms in chromium-rich Fe-Cr alloys - Ab initio results. *J. Nucl. Mater.*, **395**, 45–49.
- [26] Järvi T.T., Kuronen A., Nordlund K. and Albe K. (2009). Damage production in nanoparticles under light ion irradiation. *Phys. Rev. B*, **80**, 132101.
- [27] Tolvanen A., Buchs G., Ruffieux P., Groning P., Groning O. and Krasheninnikov A. (2009). Modifying the electronic structure of semiconducting carbon nanotubes by Ar ion irradiation. *Phys. Rev. B*, **80**, 125430.
- [28] Hulman M., Skakalova V., Krasheninnikov A. and Roth S. (2009). Effects of ion beam heating on Raman spectra of single-walled carbon nanotubes. *Appl. Phys. Lett.*, **94**, 071907.
- [29] Riikonen S., Foster A., Krasheninnikov A.V. and Nieminen R. (2009). Computational study of boron nitride nanotube synthesis: How catalyst morphology stabilizes the boron nitride bond. *Phys. Rev. B*, **80**, 155429.
- [30] Rodriguez-Manzo J., Janowska I., Pham-Huu C., Tolvanen A., Krasheninnikov A.V., Nordlund K. and Banhart F. (2009). Growth of Single-Walled Carbon Nanotubes from Sharp Metal Tips. *Small*, **5**, 2710–2715.
- [31] Harjunmaa A. and Nordlund K. (2009). Molecular dynamics simulations of Si/Ge cluster condensation. *Comp. Mater. Sci.*, **47**, 456–459.
- [32] Björkas C., Nordlund K. and Dudarev S. (2009). Modelling radiation effects using the ab-initio based tungsten and vanadium potentials. *Nucl. Instr. Meth. Phys. Res. B*, **267**, 3204–3208.

- [33] Kaila V.R.I., Johansson M.P., Sundholm D., Laakkonen L. and Wikström M. (2009). The chemistry of the Cu_B site in cytochrome *c* oxidase and the importance of its unique His–Tyr bond. *Biochim. Biophys. Acta Bioenerg.*, **1787**, 221–233.
- [34] Fliegl H., Sundholm D., Taubert S., Juselius J. and Klopper W. (2009). Magnetically Induced Current Densities in Aromatic, Antiaromatic, Homoaromatic, and Nonaromatic Hydrocarbons. *J. Phys. Chem. A*, **113**, 8668–8676.
- [35] Lehtonen O., Sundholm D., Send R. and Johansson M.P. (2009). 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**, 024301.
- [36] Send R., Sundholm D., Johansson M.P. and Pawlowski F. (2009). Excited-state potential energy surfaces of polyenes and protonated Schiff bases. *J. Chem. Theory Comput.*, **5**, 2401–2414.
- [37] Taubert S., Sundholm D. and Pichierri F. (2009). Magnetically Induced Currents in Bianthraquinodimethane-Stabilized Möbius and Hückel [16]Annulenes. *J. Org. Chem.*, **74**, 6495–6502.
- [38] Pyykkö P. and Atsumi M. (2009). Molecular Single-Bond Covalent Radii for Elements 1–118. *Chem. Eur. J.*, **15**, 186–197.
- [39] Zaleski-Ejgierd P. and Pyykkö P. (2009). Au_nHg_m Clusters: Mercury Aurides, Gold Amalgams, or van der Waals Aggregates? *J. Phys. Chem. A*, **113**, 12380–12385.
- [40] Zaleski-Ejgierd P. and Pyykkö P. (2009). Bonding analysis for sterically uncongested simple aurocarbons C_nAu_m. *Can. J. Chem.*, **87**, 798–801.
- [41] Muñliz J., Sansores L.E., Pyykkö P., Martínez A. and Salcedo R. (2009). Theoretical study on the series of [Au₃Cl₃M₂] complexes, with M = Li, Na, K, Rb, Cs. *J. Mol. Model.*, **15**, 1165–1173.
- [42] Bieron J., Froese Fischer C., Indelicato P., Jönsson P. and Pyykkö P. (2009). Complete-active-space multiconfiguration Dirac-Hartree-Fock calculations of hyperfine-structure constants of the gold atom. *Phys. Rev. A*, **79**, 052502.
- [43] Krasheninnikov A.V., Lehtinen P.O., Foster A.S., Pyykkö P. and Nieminen R.M. (2009). Embedding transition-metal atoms in graphene: Structure, bonding, and magnetism. *Phys. Rev. Lett.*, **102**, 126807.
- [44] Fernández-Torre D., Kupiainen O., Pyykkö P. and Halonen L. (2009). Long-range interactions between polar molecules and metallic surfaces: A comparison of classical and density functional theory based models. *Chem. Phys. Lett.*, **471**, 239–243.
- [45] Sumerin V., Schulz F., Nieger M., Atsumi M., Wang C., Leskelä M., Pyykkö P., Repo T. and Rieger B. (2009). Experimental and theoretical treatment of hydrogen splitting and storage in boron-nitrogen systems. *J. Organomet. Chem.*, **694**, 2654–2660.
- [46] Pyykkö P. and Atsumi M. (2009). Molecular Double-Bond Covalent Radii for Elements Li–E112. *Chem. Eur. J.*, **15**, 12770–12779.
- [47] Dognon J., Clavaguera C. and Pyykkö P. (2009). A Predicted Organometallic Series Following a 32-Electron Principle: An@C28 (An = Th, Pa⁺, U²⁺, Pu⁴⁺). *J. Am. Chem. Soc.*, **131**, 238–243.
- [48] Johansson M.P. (2009). On the Strong Ring Currents in B₁₀ and Neighboring Boron Toroids. *J. Phys. Chem. C*, **113**, 524–530.
- [49] Johansson M. and Patzschke M. (2009). Fixing the Chirality and Trapping the Transition State of Helicene with Atomic Metal Glue. *Chem. Eur. J.*, **15**, 13210–13218.
- [50] Hakala M., Nygård K., Juha Vaara M.I., Sakurai Y. and Hämäläinen K. (2009). Charge localization in alcohol isomers studied by Compton scattering. *J. Chem. Phys.*, **130**, 034506.

- [51] Hanni M., Lantto P. and Vaara J. (2009). Pairwise additivity in the nuclear magnetic resonance interactions of atomic xenon. *Phys. Chem. Chem. Phys.*, **11**, 2485–2496.
- [52] Jaszunski M. and Vaara J. (2009). ^{19}F spin-spin coupling in peri-difluoronaphthalene. *Phys. Chem. Chem. Phys.*, **11**, 4136–4140.
- [53] Liimatainen H., Pennanen T.O. and Vaara J. (2009). ^1H Chemical shifts in non-axial, paramagnetic chromium(III) complexes: Application of novel pNMR shift theory. *Can. J. Chem.*, **87**, 954–964.
- [54] Hyvärinen M., Vaara J., Goldammer A., Barbara Kutzky K.H., Kaupp M. and Straka M. (2009). Characteristic spin-orbit induced $^1\text{H}(\text{CH}_2)$ chemical shifts upon deprotonation of group 9 polyamine aqua and alcohol complexes. *J. Am. Chem. Soc.*, **131**, 11909–11918.
- [55] Ikäläinen S., Lantto P., Manninen P. and Vaara J. (2009). NMR tensors in planar hydrocarbons of increasing size. *Phys. Chem. Chem. Phys.*, **11**, 11404–11414.
- [56] Vainio M., Peltola J., Persijn S., Harren F.J.M. and Halonen L. (2009). Thermal effects in singly resonant continuous wave parametric oscillator. *Appl. Phys. B*, **94**, 411–427.
- [57] Vainio M., Siltanen M., Peltola J. and Halonen L. (2009). Continuous-wave optical parametric oscillator tuned by a diffraction grating. *Optics Express*, **17**, 7702–7707.
- [58] Stamyk K., Vaittinen O., Jaakola J., Guss J., Metsäslä M., Johanson G. and Halonen L. (2009). Background levels of HCN in human breath measured by cavity ring down spectroscopy. *Biomarkers*, **14**, 285–291.
- [59] Hänninen V., Salmi T. and Halonen L. (2009). Acceptor tunneling motion and O-H stretching vibration overtones of the water dimer. *J. Phys. Chem. A*, **113**, 7133–7137.
- [60] Salmi T., Kjaergaard H.G. and Halonen L. (2009). Calculation of overtone O-H stretching bands and intensities of the water trimer. *J. Phys. Chem. A*, **113**, 9124–9132.
- [61] Rissanen M.P., Eskola A.J., Savina E. and Timonen R.S. (2009). Kinetics of the Reactions of CH_3CH_2 , CH_3CHCl , and CH_3CCl_2 Radicals with NO_2 in the Temperature Range 221–363 K. *J. Phys. Chem. A*, **113**, 1753–1759.
- [62] Khriachtchev L., Räsänen M. and Gerber R.B. (2009). Noble-Gas Hydrides: New Chemistry at Low Temperatures. *Acc. Chem. Res.*, **42**, 183–191.
- [63] Khriachtchev L., Nikitin T., Rama Velagapudi J.L. and Novikov S. (2009). Light-emission mechanism of thermally annealed silicon-rich silicon oxide revisited: What is the role of silicon nanocrystals? *Appl. Phys. Lett.*, **94**, 043115.
- [64] Domanskaya A., Marushkevich K., Khriachtchev L. and Räsänen M. (2009). Spectroscopic study of cis-to-trans tunnelling reaction of HCOOD in rare gas matrices. *J. Chem. Phys.*, **130**, 154509.
- [65] Nikitin T., Khriachtchev L., Räsänen M. and Novikov S. (2009). Optical memory of silicon nanocrystals with submicron spatial resolution and very high thermal stability. *Appl. Phys. Lett.*, **94**, 173116.
- [66] Bochenkova A.V., Bochenkov V.E. and Khriachtchev L. (2009). HArF in solid argon revisited: Transition from unstable to stable configuration. *J. Phys. Chem. A*, **113**, 7654–7659.
- [67] Khriachtchev L., Domanskaya A., Marushkevich K., Räsänen M., Grigorenko B., Ermilov A., Andriychenko N. and Nemukhin A. (2009). Conformation-dependent chemical reaction of formic acid with an oxygen atom. *J. Phys. Chem. A*, **113**, 8143–8146.
- [68] Corani A., Domanskaya A., Khriachtchev L., Räsänen M. and Lignell A. (2009). Matrix-isolation and ab initio study of the $\text{HKrCl}\cdots\text{HCl}$ complex. *J. Phys. Chem. A*, **113**, 10687–10692.

- [69] Domanskaya A., Kobzarenko A.V., Tsivion E., Khriachtchev L., Feldman V.I., Gerber R.B. and Räsänen M. (2009). Matrix-isolation and ab initio study of HXeCCH complexed with acetylene. *Chem. Phys. Lett.*, **481**, 83–87.