MIKKO HAKALA

PUBLICATIONS 21.6.2016

Double asterisk (**) and boldface mark the ten most important publications.

Peer-reviewed scientific articles (68 publications)

1. *Theoretical and experimental study of positron annihilation with core electrons in solids*, M. Alatalo, B. Barbiellini, M. Hakala, H. Kauppinen, T. Korhonen, M. J. Puska, K. Saarinen, P. Hautojärvi, and R. M. Nieminen, Phys. Rev. B. **54**, 2397 (1996).

2. *Correlation effects for electron-positron momentum density in solids*, B. Barbiellini, M. Hakala, M. J. Puska, K. Saarinen, R. M. Nieminen, and A. A. Manuel, Phys. Rev. B. **56**, 7136 (1997).

3. *Correlation effects for positron annihilation with core and semicore electrons*, B. Barbiellini, M. J. Puska, M. Alatalo, M. Hakala, A. Harju, T. Korhonen, S. Siljamäki, T. Torsti, R. M. Nieminen, Appl. Surf. Sci. **116**, 283 (1997).

4. ** **Momentum distributions of electron-positron pairs annihilating at vacancy clusters in Si**, M. Hakala, M. J. Puska, and R. M. Nieminen, Phys. Rev. B. **57**, 7621 (1998).

5. *Microscopic identification of native donor Ga-vacancy complexes in Te-doped GaAs*, J. Gebauer, M. Lausmann, T. E. M. Staab, R. Krause-Rehberg, M. Hakala, and M. J. Puska, Phys. Rev. B. **60**, 1464 (1999).

6. *Identification of vacancy-impurity complexes in highly n-type Si*, K. Saarinen, J. Nissilä, H. Kauppinen, M. Hakala, M. J. Puska, P. Hautojärvi, and C. Corbel, Phys. Rev. Lett. **82**, 1883 (1999).

7. *The structure of vacancy-impurity complexes in highly n-type Si*, K. Saarinen, J. Nissilä, H. Kauppinen, M. Hakala, M. J. Puska, P. Hautojärvi, and C. Corbel, Physica B **273-274**, 463 (1999).

8. *Observation of Ga vacancies and negative ions in undoped and Mg-doped GaN bulk crystals*, K. Saarinen, J. Nissilä, J. Oila, V. Ranki, M. Hakala, M. J. Puska, P. Hautojärvi, J. Likonen, T. Suski, I. Grzegory, B. Lucznik, and S. Porowksi, Physica B **273-274**, 33 (1999).

9. *Theoretical studies of interstitial boron defects in silicon*, M. Hakala, M. J. Puska, R. M. Nieminen, Physica B **273-274**, 268 (1999).

10. ** **First-principles calculations of interstitial boron in silicon**, M. Hakala, M. J. Puska, and R. M. Nieminen, Phys. Rev. B **61**, 8155 (2000).

11. *Irradiation experiment revisited - Stability and positron lifetime of large vacancy clusters in silicon*,
T. E. M. Staab, M. J. Puska, M. Hakala, A. Sieck, M. Haugk, T. Frauenheim, and H. S. Leipner, Mater. Sci. Forum **363-365**, 135 (2001).

12. *Native defects and self-diffusion in GaSb*,
M. Hakala, M. J. Puska and R. M. Nieminen, J. Appl. Phys. **91**, 4988 (2002).

13. *Scattering effects in a positron lifetime beam line*,
A. Laakso, M. O. Hakala, A. Pelli, K. Rytsölä, and K. Saarinen, Mater. Sci. Forum. **445**, 489 (2004).

14. *Compton profiles for water and mixed water-neon clusters: A measure of coordination*,
M. Hakala, S. Huotari, K. Hämäläinen, S. Manninen, Ph. Wernet, A. Nilsson, and L. G. M. Pettersson, Phys. Rev. B **70**, 125413 (2004).

15. *Electron emission from solids under electron irradiation: a Monte Carlo study*,
M. Hakala, C. Corbel and R. M. Nieminen, J. Phys. D **38**, 711 (2005).

16. *Calculation of valence electron momentum densities using the projector augmented-wave method*,
I. Makkonen, M. Hakala, and M. J. Puska, J. Phys. Chem. Solids **66**, 1128 (2005).

17. *Modeling the momentum distributions of annihilating electron-positron pairs in solids*,
I. Makkonen, M. Hakala, and M. J. Puska, Phys. Rev. B **73**, 035103 (2006).

18. *Intra- and intermolecular effects in the Compton profile of water*,
M. Hakala, K. Nygård, S. Manninen, L. G. M. Pettersson and K. Hämäläinen, Phys. Rev. B **73** 035432 (2006).

19. *Ion hydration studied by X-ray Compton scattering*,
K. Nygård, M. Hakala, S. Manninen, K. Hämäläinen, M. Itou, A. Andrejczuk, and Y. Sakurai, Phys. Rev. B **73** 024208 (2006).

20. *First-principles calculation of positron states and annihilation at defects in semiconductors*,
I. Makkonen, M. Hakala, and M. J. Puska, Physica B **376-377**, 971 (2006).

21. *Electronic stucture of methane hydrate studied by Compton scattering*,
C. Sternemann, S. Huotari, M. Hakala, M. Paulus, M. Volmer, C. Gutt, T. Buslaps, N. Hiraoka, D. D. Klug, K. Hämäläinen, M. Tolan, and J. S. Tse, Phys. Rev. B **73**, 195104 (2006).

22. **** Gold as intermolecular glue: a predicted planar triaurotriazine, $C_3Au_3N_3$, isomer of gold cyanide**,
M. O. Hakala and P. Pyykkö, Chem. Commun., 2890 (2006).

23. *Correlation of hydrogen bond lengths and angles in liquid water based on Compton scattering*,
M. Hakala, K. Nygård, S. Manninen, S. Huotari, T. Buslaps, A. Nilsson, L. G. M. Pettersson, and K. Hämäläinen, J. Chem. Phys. **125**, 084504 (2006).

24. *Compton scattering study of water versus ice Ih: Intra- and intermolecular structure*, K. Nygård, M. Hakala, S. Manninen, A. Andrejczuk, M. Itou, Y. Sakurai, L. G. M. Pettersson and K. Hämäläinen, Phys. Rev. E **74**, 031503 (2006).

25. *Isotope quantum effects in the Compton profile of water*, K. Nygård, M. Hakala, T. Pylkkänen, S. Mannine, T. Buslaps, M. Itou, A. Andrejczuk, Y. Sakurai, M. Odelius and K. Hämäläinen, J. Chem. Phys. **126**, 154508 (2007).

26. *Gold as intermolecular glue: a theoretical study of nanostrips based on quinoline-type monomers*, P. Pyykkö, M. O. Hakala and P. Zaleski-Ejgierd, Phys. Chem. Chem. Phys. **9**, 3025 (2007).

27. *Comparison of chain versus sheet crystal structures for the cyanides MCN (M=Cu-Au) and dicarbides MC_2 (M=Be-Ba,Zn-Hg)*, P. Zaleski-Ejgierd, M. Hakala, and P. Pyykkö, Phys. Rev. B **76**, 094104 (2007).

28. *Configurational energetics in ice Ih probed by Compton scattering*, K. Nygård, M. Hakala, S. Manninen, M. Itou, Y. Sakurai and K. Hämäläinen, Phys. Rev. Lett. **99**, 197401 (2007).

29. **** Density functional study of X-ray Raman scattering from aromatic hydrocarbons and polyfluorene**, A. Sakko, M. Hakala, J. A. Soininen, and K. Hämäläinen, Phys. Rev. B **76**, 205115 (2007).

30. *Development of a ReaxFF description for gold*, T. T. Järvi, A. Kuronen, M. Hakala, K. Nordlund, A. C. T. van Duin, W. A. Goddard III, and T. Jacob, Eur. Phys. J. B **66**, 75 (2008).

31. *Charge localization in alcohol isomers studied by Compton scattering*, M. Hakala, K. Nygård, J. Vaara, M. Itou, Y. Sakurai and K. Hämäläinen, J. Chem. Phys. **130**, 034506 (2009).

32. **** Structure of Liquid Linear Alcohols**, J. S. Lehtola, M. Hakala and K. Hämäläinen, J. Phys. Chem. B **114**, 6426 (2010).

33. *Role of non-hydrogen-bonded molecules in the oxygen K-edge spectrum in ice*, T. Pylkkänen, V. M. Giordano, J.-C. Chervin, A. Sakko, M. Hakala, J. A. Soininen, K. Hämäläinen, G. Monaco and S. Huotari, J. Phys. Chem. B **114**, 3804 (2010).

34. *Amorphous defect clusters of pure Si and type inversion in Si detectors*, E. Holmström, K. Nordlund and M. Hakala, Phys. Rev. B **82**, 104111 (2010).

35. *Anomalous Energetics in Tetrahydrofuran Clathrate Hydrate Revealed by X-ray Compton Scattering*, F. Lehmkühler, A. Sakko, C. Sternemann, M. Hakala, K. Nygård, Ch. J. Sahle, S. Galambosi, I. Steinke, S. Tiemeyer, A. Nyrow, T. Buslaps, D. Pontoni, M. Tolan, and K. Hämäläinen, J. Phys. Chem. Lett. **1**, 2832 (2010).

36. *Universal Signature of Hydrogen Bonding in the Oxygen K-Edge Spectrum of Alcohols*, T. Pylkkänen, J. Lehtola, M. Hakala, A. Sakko, G. Monaco, S. Huotari, and K. Hämäläinen, J. Phys. Chem. B **114**, 13076 (2010).

37. **** Time-dependent density functional approach for the calculation of inelastic x-ray scattering spectra of molecules**, A. Sakko, A. Rubio, M. Hakala, and K. Hämäläinen, J. Chem. Phys. **133**, 174111 (2010).

38. *Nuclear magnetic resonance parameters in water dimer*, T. S. Pennanen, P. Lantto, M. Hakala and J. Vaara, Theor. Chem. Acc. **129**, 313 (2011).

39. *Experimental and computational study of crystalline formic acid composed of the higher-energy cis conformer*, M. Hakala, K. Marushkevich, L. Khriachtchev, K. Hämäläinen, and M. Räsänen, J. Chem. Phys. **134**, 054506 (2011).

40. *Calculation of isotropic Compton profiles with Gaussian basis sets*, J. Lehtola, M. Hakala, J. Vaara, and K. Hämäläinen, Phys. Chem. Chem. Phys. **13**, 5630 (2011).

41. *Inelastic x-ray scattering and vibrational effects at the K-edges of gaseous N_2, N_2O, and CO_2*, A. Sakko, S. Galambosi, J. Inkinen, T. Pylkkänen, M. Hakala, S. Huotari, and K. Hämäläinen, Phys. Chem. Chem. Phys. **13**, 11678 (2011).

42. *Reexamining the Lyman-Birge-Hopfield Band of N_2*, J. A. Bradley, A. Sakko, G. T. Seidler, A. Rubio, M. Hakala, K. Hämäläinen, G. Cooper, A. P. Hitchcock, K. Schlimmer, and K. P. Nagle, Phys. Rev. A **84**, 022510 (2011).

43. *Temperature Induced Structural Changes of Tetrahydrofuran Clathrate and of the Liquid Water/Tetrahydrofuran Mixture*, F. Lehmkühler, A. Sakko, I. Steinke, C. Sternemann, M. Hakala, C. J. Sahle, T. Buslaps, L. Simonelli, S. Galambosi, M. Paulus, T. Pylkknen, M. Tolan, and K. Hämäläinen, J. Phys. Chem. C **115**, 21009 (2011).

44. **** Measurement of two solvation regimes in water-ethanol mixtures using x-ray Compton scattering**, I. Juurinen, K. Nakahara, N. Ando, T. Nishiumi, H. Seta, N. Yoshida, T. Morinaga, M. Itou, T. Ninomiya, Y. Sakurai, E. Salonen, K. Nordlund, K. Hämäläinen, and M. Hakala, Phys. Rev. Lett. **107**, 197401 (2011).

45. *Temperature dependence of the near-edge spectrum of water*, T. Pylkkänen, A. Sakko, M. Hakala, K. Hämäläinen, G. Monaco, and S. Huotari, J. Phys. Chem. B **115**, 14544 (2011).

46. *ERKALE - A Flexible Program Package for X-ray Properties of Atoms and Molecules*, J. Lehtola, M. Hakala, A. Sakko, and K. Hämäläinen, J. Comput. Chem. **33**, 1572 (2012).

47. *Completeness-optimized basis sets: Application to ground-state electron momentum densities*,
J. Lehtola, P. Manninen, M. Hakala, and K. Hämäläinen, J. Chem. Phys. **137**, 104105 (2012).

48. *Contraction of completeness-optimized basis sets: Application to ground-state electron momentum densities*,
S. S. Lehtola, P. Manninen, M. Hakala, and K. Hämäläinen, J. Chem. Phys. **138**, 044109 (2013).

49. ** **Microscopic structure of water at elevated pressures and temperatures**,
C. J. Sahle, C. Sternemann, C. Schmidt, S. S. Lehtola, S. Jahn, L. Simonelli, S. Huotari, M. Hakala, T. Pylkkänen, A. Nyrow, K. Mende, M. Tolan, K. Hämäläinen, and M. Wilke, Proc. Natl. Acad. Sci. USA **110**, 6301 (2013).

50. *Temperature dependence of CO2 and N2 core-electron excitation spectra at high pressure*,
J. Inkinen, A. Sakko, K. O. Ruotsalainen, T. Pylkkänen, J. Niskanen, S. Galambosi, M. Hakala, G. Monaco, S. Huotari, and K. Hämäläinen, Phys. Chem. Chem. Phys. **15**, 9231 (2013)

51. *Local changes of work function near rough features on Cu surfaces operated under high external electric field*,
F. Djurabekova, A. Ruzibaev, E. Holmström, S. Parviainen, and M. Hakala, J. Appl. Phys. **114**, 243302 (2013).

52. *Saturation Behaviour in X-ray Raman Scattering Spectra of Aqueous LiCl*,
I. Juurinen, T. Pylkkänen, K. O. Ruotsalainen, C. Sahle, G. Monaco, K. Hämäläinen, S. Huotari, and M. Hakala, J. Phys. Chem. B **117**, 16506 (2013)

53. *Interplay between Temperature-Activated Vibrations and Nondipolar Effects in the Valence Excitations of the CO2 Molecule*,
J. Inkinen, J. Niskanen, A. Sakko, K. O. Ruotsalainen, T. Pylkkänen, S. Galambosi, M. Hakala, G. Monaco, K. Hämäläinen, and S. Huotari, J. Phys. Chem. A **118**, 3288 (2014)

54. *Crystal-field excitations in NiO under high pressure studied by resonant inelastic x-ray scattering*,
S. Huotari, L. Simonelli, V. M. Giordano, A. E. Rintala, Ch. J. Sahle, M. Hakala, P. Glatzel, R. Verbeni, and G. Monaco, J. Phys.: Condens. Matter **26**, 135501 (2014)

55. ** **Molecular-Level Changes of Aqueous Poly(N-isopropylacrylamide) in Phase Transition**,
I. Juurinen, S. Galambosi, A. G. Anghelescu-Hakala, J. Koskelo, V. Honkimäki, K. Hämäläinen, S. Huotari, and M. Hakala, J. Phys. Chem. B **118**, 5518 (2014)

56. *Effect of the Hydrophobic Alcohol Chain Length on the Hydrogen-Bond Network of Water*,
I. Juurinen, T. Pylkkänen, Ch. J. Sahle, L. Simonelli, K. Hämäläinen, S. Huotari, and M. Hakala, J. Phys. Chem. B **118**, 8750 (2014)

57. **** Multi-intermediate-band character of Ti-substituted CuGaS2: Implications for photovoltaic applications**,
J. Hashemi, A. Akbari, S. Huotari, and M. Hakala, Phys. Rev. B **90**, 075154 (2014)

58. *Intra- and intermolecular effects on the Compton profile of the ionic liquid 1,3-dimethylimidazolium chloride*,
J. Koskelo, I. Juurinen, K. O. Ruotsalainen, M. McGrath, I.-F. Kuo, S. Lehtola, S. Galambosi, K. Hämäläinen, S. Huotari and M. Hakala, The Journal of Chemical Physics **141**, 244505 (2014)

59. *Identification of the dye adsorption modes in dye-sensitised solar cells with X-ray spectroscopy techniques: a computational study*,
A. Akbari, J. Hashemi, J. Niskanen, S. Huotari, and M. Hakala, Phys. Chem. Chem. Phys. **17**, 10849 (2015)

60. *Inelastic x-ray scattering in heterostructures: electronic excitations in LaAlO3/SrTiO3*,
K. O. Ruotsalainen, C. J. Sahle, T. Ritschel, J. Geck, M. Hosoda, C. Bell, Y. Hikita, H. Y. Hwang, T. T. Fister, R. A. Gordon, K. Hämäläinen, M. Hakala, and S. Huotari, J. Phys.: Condens. Matter **27**, 335501 (2015)

61. *Exciton energy-momentum map of hexagonal boron nitride*,
G. Fugallo, M. Aramini, J. Koskelo, K. Watanabe, T. Taniguchi, M. Hakala, S. Huotari, M. Gatti, and F. Sottile, Phys. Rev. B **92**, 165122 (2015)

62. *Protonation Dynamics and Hydrogen Bonding in Aqueous Sulfuric Acid*,
J. Niskanen, C.J. Sahle, I. Juurinen, J. Koskelo, S. Lehtola, R. Verbeni, H. Müller, M. Hakala, and S. Huotari, J. Phys. Chem. B **119**, 11732 (2015)

63. *X-ray induced dimerization of cinnamic acid: Time-resolved inelastic X-ray scattering study*,
J. Inkinen, J. Niskanen, T. Talka, C. Sahle, H. Müller, L. Khriachchev, J. Hashemi, A. Akbari, M. Hakala and S. Huotari, Sci. Rep. **5**, 15851 (2015)

64. *Probing the thermal stability and decomposition mechanism of a magnesium-fullerene polymer via X-ray Raman spectroscopy, X-ray diffraction and molecular dynamics simulations*,
M. Aramini, J. Niskanen, C. Cavallari, D. Pontiroli, A. Musazay, M. Krisch, M. Hakala and S. Huotari, Phys. Chem. Chem. Phys. **18**, 5366 (2016)

65. *Sulphur Kb emission spectra reveal protonation states of aqueous sulfuric acid*,
J. Niskanen, C.J. Sahle, K. O. Ruotsalainen, H. Müller, M. Kavcic, M. Zitnik, K. Bucar, M. Petric, M. Hakala and S. Huotari, Sci. Rep. **6**, 21012 (2016)

66. *Resonant X-ray emission with a standing wave excitation*,
K.O. Ruotsalainen, A.-P. Honkanen, S.P. Collins, G. Monaco, Moretti M. Sala, M. Krisch, K. Hämäläinen, M. Hakala and S. Huotari, **6**, 22648 (2016)

67. *Intramolecular structure and energetics in supercooled water down to 255 K*,
F. Lehmkühler, Y. Forov, T. Bning, C.J. Sahle, I. Steinke, K. Julius, T. Buslaps, M. Tolan, M. Hakala and C. Sternemann, Phys. Chem. Chem. Phys. **18**, 6925 (2016)

68. *First-principles analysis of the intermediate band in CuGa(1-x)FexS2*, J. Koskelo, J. Hashemi, S. Huotari and M. Hakala, Phys. Rev. B **93**, 165204 (2016)

Non-refereed scientific articles

1. *First-Principles Calculations of Positron Annihilation in Solids*, B. Barbiellini, M. Hakala, R. M. Nieminen, and M. J. Puska, Proceedings of the MRS Fall Meeting, Boston, USA, 1999.

Publications intended for the general public

1. *Synkrotronisäteily paljastaa aineen rakenteen*, K. Hämäläinen and M. Hakala, Radio interview (in Finnish), Finnish Broadcasting Company (YLE), 25.1.2006
2. *Approach to Cold Heat-Storage Mechanism of Ice*, K. Hämäläinen, S. Manninen, K. Nygård, M. Hakala, M. Itou and Y. Sakurai, Press release, SPring-8, Japan, 8.11.2007.
3. *Uutta tietoa veden lämpöominaisuuksista röntgensironnalla*, Press release (in Finnish), The Finnish News Agency (STT), 14.11.2007.
4. *Configurational energetics in ice Ih probed by Compton scattering*, K. Nygård, M. Hakala, and K. Hämäläinen, SPring-8 Research Frontiers 2007, Japan.
5. *New information on thermal properties of water through X-ray scattering technique*, CSC News 1/2008, p. 9.
6. *Nestemäisten lineaaristen alkoholien rakenneanalyysi*, CSC Ajankohtaista (in Finnish), 17.5.2010.
7. *Striving for the best possible accuracy in models*, interview, CSC News 1/2011, p. 4.
8. *Molekyylitason rakennetutkimusta röntgenmenetelmin*, M. Hakala, Arkhimedes **1**, 14 (2012).
9. *Ethanol-water structures at the microscopic level studied by X-ray Compton scattering: extreme sensitivity to geometries*, M. Hakala, I. Juurinen and K. Nakahara, SPring-8 Research Frontiers 2011, Japan.
10. *Scientists probe atomic structure and dynamics of water under deep Earth extreme pressure and temperature conditions*, C. J. Sahle, C. Sternemann, C. Schmidt, S. S. Lehtola, S. Jahn, L. Simonelli, S. Huotari, M. Hakala, T. Pylkkänen, A. Nyrow, K. Mende, M. Tolan, K. Hämäläinen, and M. Wilke, ESRF News 8.3.2013
11. *Microscopic structure of water under conditions of the Earth's crust and mantle*, C. J. Sahle, C. Sternemann, C. Schmidt, S. S. Lehtola, S. Jahn, L. Simonelli, S. Huotari, M. Hakala, T. Pylkkänen, A. Nyrow, K. Mende, M. Tolan, K. Hämäläinen, and M. Wilke, ESRF Highlights 2013

Theses

1. Master's thesis: *Computational Scheme for Core-Electron Annihilation in Solids*, Helsinki University of Technology (1996)

2. Doctoral dissertation: *Defect Complexes in Silicon: Electronic Structures and Positron Annihilation*, Helsinki University of Technology (2001)

Invited talks

1. *X-ray Compton scattering as a probe of hydrogen bonds and local coordination in water*
Stockholm Discussion Meeting, 14.-16.6.2006, Albanova University Center, Stockholm University, Sweden

2. *Hydrogen Bonds in Water and Aqueous Systems Studied by Compton Scattering and DFT Calculations*
Sagamore XV Conference, 13.-18.8.2006, University of Warwick, Warwickshire, United Kingdom

3. *What Compton Scattering Tells about the Intra- and Intermolecular structure of Water*
Bunsen-Kolloquium: Chemical Bonding in Position, Momentum, and Phase Space, 5.-6.2.2007, Univ. Konstanz, Germany

4. *Compton scattering as a probe of hydrogen bonds and molecular structure of aqueous systems*
6th International Conference on Inelastic X-ray Scattering, 7.-11.5.2007, Awaji, Japan

5. *Liquids and molecular systems by X-ray Compton and Raman scattering*
5th Summer School for Synchrotron Radiation Users, 11.-13.8.2008, Kuortane, Finland

6. *Electronic properties of molecular structures by inelastic X-ray scattering*
XIV International Workshop on Quantum Systems in Chemistry and Physics, 13.-19.9.2009, Madrid, Spain

7. *Sub-nanometer properties of materials by theoretical and experimental Compton scattering*
Sagamore XVII Conference, 15.-20.7.2012, Kitayuzawa, Hokkai-do, Japan

8. *Electronic structure and x-ray properties*
Summer School on Novel Approaches to Electronic Structure Theory, 15.-17.8.2012, Tampere, Finland

9. *Structure of water studied by inelastic x-ray scattering*
7th International Discussion Meeting on Relaxations in Complex Systems, 21.-26.7.2013, Barcelona, Spain

10. *Non-resonant inelastic x-ray scattering in molecular systems: sensitivity to geometries*
8th International Conference on Inelastic X-ray Scattering, 11.-16.8.2013, Menlo Park, CA, USA

11. *Inelastic x-ray scattering spectroscopy*
    Winter School in Theoretical Chemistry 2013: Theoretical Spectroscopy, 18.12.2013, Helsinki, Finland

12. *Social media - Possibilies to popularize history*
    Helsinki Summer University, 21.6.2016, Helsinki, Finland