

## 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. Porowski, 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. Rytölä, 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 structure 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*,  
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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 ( $M=\text{Cu-Au}$ ) and dicarbides  $\text{MC}_2$  ( $M=\text{Be-Ba, Zn-Hg}$ )*, 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. Lehmkuhler, 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. Lehmkuhler, 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*,  
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48. *Contraction of completeness-optimized basis sets: Application to ground-state electron momentum densities*,  
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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 CO<sub>2</sub> and N<sub>2</sub> 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 CO<sub>2</sub> 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. Koskela, 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 CuGaS<sub>2</sub>: 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,*  
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  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 LaAlO<sub>3</sub>/SrTiO<sub>3</sub>,*  
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,*  
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  62. *Protonation Dynamics and Hydrogen Bonding in Aqueous Sulfuric Acid,*  
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  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 K $\beta$  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. Lehmkuhler, 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)
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68. *First-principles analysis of the intermediate band in  $\text{CuGa}(1-x)\text{Fe}_x\text{S}_2$* , J. Koskelo, J. Hashemi, S. Huotari and M. Hakala, Phys. Rev. B **93**, 165204 (2016)
69. *First principles modeling of perovskite solar cells based on  $\text{TiO}_2$  and  $\text{Al}_2\text{O}_3$ : Stability and Interfacial Electronic Structure*, A. Akbari, J. Hashemi, E. Mosconi, F. De Angelis and M. Hakala, submitted to J. Phys. Chem. Lett. (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. *Molekyylistason 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 - Possibilities to popularize history*  
Helsinki Summer University, 21.6.2016, Helsinki, Finland