

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).
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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*,  
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12. *Native defects and self-diffusion in GaSb*,  
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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*,  
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16. *Calculation of valence electron momentum densities using the projector augmented-wave method*,  
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17. *Modeling the momentum distributions of annihilating electron-positron pairs in solids*,  
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18. *Intra- and intermolecular effects in the Compton profile of water*,  
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20. *First-principles calculation of positron states and annihilation at defects in semiconductors*,  
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22. **\*\* Gold as intermolecular glue: a predicted planar triaurotriazine,  $C_3Au_3N_3$ , isomer of gold cyanide**,  
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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).
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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).
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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).

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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).
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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).
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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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63. *X-ray induced dimerization of cinnamic acid: Time-resolved inelastic X-ray scattering study,*  
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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,*  
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68. *First-principles analysis of the intermediate band in CuGa(1-x)FeS<sub>2</sub>*,  
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. Ny-  
gård, 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),  
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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),  
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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  
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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.  
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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