MIKKO HAKALA

PUBLICATIONS 16.11.2017

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

A1 Peer-reviewed scientific articles

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). www

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5. *Microscopic identification of native donor Ga-vacancy complexes in Te-doped GaAs*,
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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). www

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**,
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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*,
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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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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).

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72. *Hydrogen adsorption on MoS2-surfaces: a DFT study on preferential sites and the effect of sulfur and hydrogen coverage*,
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B3 Non-refereed scientific articles

1. *First-Principles Calculations of Positron Annihilation in Solids*,
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E1 Publications intended for the general public

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G 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)