

Curriculum Vitae

René WINDIKS

Personal Dates

Date of birth	June 9, 1971
Place of birth	Berlin, Germany
Nationality	German

Address Office

Windiks Consulting	Phone:	+41 56 282 04 64
Dorfstrasse 63B	E-Mail:	windik@swissonline.ch
5417 Untersiggenthal	Web:	http://homepage.swissonline.ch/windik/
Switzerland		

Education

1995–2000	PhD (Dr. rer. nat.) , July 2000, Humboldt University Berlin, Department of Chemistry with <i>magna cum laude</i> . Thesis title: <i>Paramagnetic Na_4^{3+} guest clusters embedded in sodalite hosts: density functional calculations of hyperfine interactions and magnetic couplings</i> . Thesis Adviser: Prof. Joachim Sauer.
1994–1995	Diploma in Chemistry (Dipl. Chem.), July 1995, Humboldt University Berlin, Department of Chemistry with <i>cum laude</i> (gut). Thesis title: <i>Suitability of density functional methods to describe hydrogen bonds of small molecules</i> . Diploma Adviser: Prof. Joachim Sauer
1990–1994	Study of Chemistry at the Technical University Berlin, Department of Chemistry

Professional Activities

2006–present	Scientific Consultant of <i>Materials Designs. Inc.</i> , USA
2006	Launching the Enterprise <i>Windiks Consulting</i> , CH
2004–2006	Postdoctoral Fellow at <i>Materials Design s.a.r.l.</i> , F
2000–2004	Postdoctoral Fellow, <i>Paul Scherrer Institute</i> , CH

Scholarships and Awards

2004–2006	Participant in the European “Research and Training Network” (RTN) “Psi-k f-electron”
2001–2004	Postdoctoral Fellowship from the Swiss National Fund for Research (SNF)
1995–2000	Participant of the Priority Programme ' <i>Host-guest interactions</i> ' of the German Research Foundation (DFG)
1994	Klaus-Koch Award, Technical University Berlin

Research Fields

- Ab-initio computation of electronic properties of f-electron materials
(collaboration with the group of A. Georges, École Polytechnique Palaiseau, France)
- Density functional molecular dynamics simulations of hydroxy apatite nucleation on silica based glass surfaces
- Development of the density functional computer program DMol³: implementation of advanced molecular dynamics algorithms
(collaboration with B. Delley, Paul Scherrer Institute, Switzerland)
- Molecular modeling of ferroelectric thin films on insulators
(collaboration with P. Willmot, Paul Scherrer Institute, Switzerland)
- Structural and electronic properties of haloform-intercalated fullerenes
(collaboration with A. Bill and B. Delley, Paul Scherrer Institute, Switzerland, and V. Z. Kresin, University of California, Berkeley California, USA)
- Host-guest interactions in zeolites

Languages

German (mother tongue), English: fluent

Publications

1. R. Windiks and J. Sauer, *Sodium doped sodium sodalite: magnetic coupling between F centers and hyperfine interactions with framework atoms*, Phys. Chem. Chem. Phys., **1**(18), 4505 (1999).
2. R. Windiks and J. Sauer, *Electronic structure and magnetic coupling in sodium electro sodalite. All-electron density functional calculations*, J. Chem. Phys., **113**(13), 5466 (2000).
3. A. Bill, R. Windiks, B. Delley, and V. Z. Kresin, *High-temperature superconductivity in intercalated molecular C₆₀/CHX₃ (X = Cl, Br, I)*, Int. J. Mod. Phys. B, **16**, 1533 (2002).
4. R. Windiks, A. Bill, B. Delley, and V. Z. Kresin, *Crystal structures and electronic properties of haloform-intercalated C₆₀ materials*, Phys. Rev. B, **66**, 195418 (2002).
5. R. Windiks, A. Bill, B. Delley, and V. Z. Kresin, *Crystal structures and electronic properties of haloform-intercalated C₆₀ materials*, Virt. Nanosc. Sci. Techn., **6** (2002).
6. R. Windiks and B. Delley, *Massive thermostating in density functional molecular dynamics simulations*, J. Chem. Phys., **119**(5), 2481 (2003).
7. J. Sauer and R. Windiks, in *Host-guest-systems based on nanoporous crystals*, edited by F. Laeri, F. Schüth, U. Simon, and M. Wark (Wiley-VCH, Heidelberg, 2003).
8. P. R. Willmott, R. Herger, B. D. Patterson, and R. Windiks, *Experimental and theoretical study of the strong dependence of the microstructural properties of Sr_xBa_{1-x}Nb₂O₆ thin films as a function of their composition*, Phys. Rev. B **71**, 144114 (2005).

Conference, Workshop and Seminar Contributions

- *Chromatic properties of pure and alkali-doped cerium sulfides: beyond the local density approximation*, 1st Int. Symposium on Structure-Property Relationships in Solid State Materials, Bordeaux, France, June 2006. **(Poster)**
- *Optical properties of pure and alkali-doped cerium sulfides: beyond the local density approximation*, Ψ_k 2005 Conference, Schäßisch-Gmünd, Germany, September 2005. **(Poster)**
- *Density functional calculations of the optical properties of rare earth compounds*, 11th Int. Conference on the Applications of Density Functional Theory in Chemistry and Physics, Geneva, Switzerland, September 2005. **(Poster)**
- *Modeling of calcium phosphate nucleation on bioactive silica glasses and glass ceramics*, Molecular Design s.a.r.l., Le Mans, France, May 2004. **(invited talk)**

- *Massive thermostating in isothermal density functional molecular dynamics simulations*, International Conference on Materials for Advanced Technologies, Singapore, December 2003. (**poster**)
- *First principles molecular dynamics simulations with the DMol³ approach*, Swiss Center for Scientific Computing, Switzerland, April 2003. (**invited talk**)
- *Molecular modeling of bone formation on bioactive materials*, Computational Biophysics: Integrating Theoretical Physics and Biology, San Feliu de Guixols, Spain, September 2002. (**poster**)
- *Molecular modeling of bone formation on bioactive materials*, 6th World Congress of Theoretically Oriented Chemists, Lugano, Switzerland, August 2002. (**poster**)
- Summer School of the NATO Advanced Study Institute: Computational Materials Science, Il Ciocco (Lucca) Italy, September 2001 (**poster**).
- *Sodium doped sodium sodalite: calculations of magnetic coupling between paramagnetic Na₄³⁺ clusters and hyperfine interactions with framework nuclei*, 100th Anniversary of the Chemistry Department, Humboldt University, Berlin, Germany, June 2000. (**poster**)
- *Sodium doped sodium sodalite: calculations of magnetic coupling between paramagnetic Na₄³⁺ clusters and hyperfine interactions with framework nuclei*, Paul Scherrer Institute, Switzerland, October 1999. (**invited talk**)
- *Sodium doped sodium sodalite: magnetic coupling between f centers and hyperfine interactions with framework atoms*, IUPAC Congress and Annual Meeting of the Association of German Chemists (GDCh), Berlin, Germany, August 1999. (**poster**)
- *Density functional calculations on sodium doped sodium sodalite*, International Conference on Quantum Chemical Calculations of NMR and EPR Parameters, Bratislava, Slovak Republic, September 1998. (**poster**)
- *Eignung von DFT-Methoden zur Beschreibung von H-Brückenbindungen*, DFT-Workshop, Quantum Chemistry Research Unit of the Max-Planck Society at the Humboldt-University, Berlin, Germany, May 1995. (**contributed talk**)