



Curriculum Vitae

## SIEGFRIED HÖFINGER

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### CONTACT INFORMATION

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### PERSONAL INFORMATION

Date of Birth:

October 29, 1968

Place of Birth:

Steyr, Austria

Citizenship:

Austrian

Marital Status:

unmarried, no children

### EDUCATION, EMPLOYMENT

1988-1996

MS in Biochemistry  
University of Vienna, Austria  
Supervisor: Prof. Othmar Steinhauser, Institute for  
Theoretical Chemistry

1996-1998

PhD in Theoretical Chemistry  
University of Vienna, Austria  
Supervisor: Prof. Othmar Steinhauser, Institute for  
Theoretical Chemistry  
Collaboration with the Research Institute for Software  
Technology, University of Salzburg, Prof. Peter Zinterhof

11/1998-10/1999

Postdoc, Biophysical Chemistry  
Institute de Génétique et de Biologie Moléculaire et  
Cellulaire, Strasbourg, France  
Collaboration with the Institute for Theoretical Chem-  
istry, University of Vienna  
Supervisor: Prof. Thomas Simonson

- 11/1999-06/2000**  
Research Assistant, Molecular Dynamics and Biomolecular Simulation  
Institute for Theoretical Chemistry and Structural Biology, University of Vienna, Austria  
Collaboration with the Institute for Graphics and Parallel Processing, University of Linz, Prof. Dieter Kranzlmüller and Prof. Jens Volkert
- 07/2000-09/2001**  
Postdoc, Carbon Nanomaterials  
University of Bologna, Italy  
Dipartimento di Chimica "G. Ciamician"  
Supervisor: Prof. Francesco Zerbetto
- 10/2001-10/2004**  
Industrial Postdoc, Medicinal Chemistry  
Novartis Institutes for BioMedical Research, Vienna, Austria  
Learning the basic principles of the drug discovery process, project support, exploring the potential of a novel computer hardware - MD-GRAPE-2;
- 11/2004-08/2005**  
Head of the Laboratory for Quantum Chemical Calculations  
Novartis Institutes for BioMedical Research, Vienna, Austria  
Cheminformatics assistance, compound solution properties, project support, developmental as well as support duties;
- 09/2005**  
Research Volunteer, Molecular Dynamics and Biomolecular Simulations  
Department of Biomolecular Structural Chemistry, University of Vienna, Austria
- 10/2005**  
Visiting Scientist, Computational Biology and Biophysics  
Forschungszentrum Jülich  
John von Neumann Institute for Computing
- 11/2005-09/2007**  
NIH Research Scholar, Computational Nano - and Biophysics  
Department of Physics  
Michigan Technological University, USA  
Protein Folding, Hydrophobicity, Continuum Electrostatics, High Performance Computing
- 10/2007-03/2008**  
Visiting Scientist, Computational Biology and Biophysics  
Forschungszentrum Jülich  
John von Neumann Institute for Computing  
Protein Folding, Hydrophobicity, Continuum Electrostatics, High Performance Computing

04/2008-07/2008	HPC Europa++ Fellow CINECA, Bologna, ITALY High Performance Computing, Hydrophobicity
07/2008-11/2009	co.co.pro. INSTM Università di Bologna, ITALY Applied Computational Biophysical Chemistry
since 11/2009	Assegnista di ricerca Università di Bologna, ITALY Applied Computational Biophysical Chemistry
since 11/2007	Adjunct Assistant Professor of Physics Michigan Technological University Biophysics, Heterogeneous Environments, Continuum Electrostatics, High Performance Computing

## PROFESSIONAL QUALIFICATIONS

- Membrane-Associated Biochemistry Protein integration into and passage across membranes (signal peptides), IL4-Receptor signaling, Pleckstrin Homology domains (characterization and functional study); 4 years of experience of working in an industrial set-up on drug discovery projects;
- Medicinal Chemistry Polar and non-polar contributions (with particular interest in parameter-free descriptions), the hydrophobic effect;
- Solvation Effects Program development of Hartree Fock as well as DFT methods, familiarity with Gaussian 03/98/94, Jaguar, Mopac, AIMPAC;
- Quantum Chemistry Free energy calculations, molecular dynamics, replica exchange MD, TINKER, AMBER;
- Molecular Mechanics Implicit solvation models for MD and QM;
- Continuum Electrostatics High performance implementation on the GPU as well as on special purpose hardware MD-GRAPE-2/3 for very fast enhanced Poisson-Boltzmann calculations → <http://84.113.253.84/~polch>
- GPUs & ASICs in Science C, Fortran, CUDA, MPI, PVM, BLAS, LAPACK, ATLAS on various supercomputing architectures;
- High Performance Computing Linux/UNIX, scripting enthusiast, html, CGI, PHP, cross-compiling, basic handling of Windows-systems;
- System Administration English (profound knowledge)
- Languages French (basic communication skills)
- Italian (basic communication skills)
- German (native language)

## TEACHING

MTU Physics Course PH4390

**Computational Methods in Physics (Fall 2006)**

## AWARDS & GRANTS

1999	Kurt Gödel scholarship for studies abroad granted by the Austrian Ministry of Science and Transport
2001	Novartis IK@N Bright Idea Award 2001, "ASIC in Molecular Modelling"
2004	HPC Europa grant to access the Pan-European Research Infrastructure for High Performance Computing; 2 weeks research stay at CINECA
2008	HPC-Europa++ Transnational Access programme; 3 months research stay at CINECA, large scale computational study on solvation of hydrophobic particles (236 kh of CPU time, AMD Opteron(tm) 2216 HE dual-core 2.4 GHz)
2009	HPC-Europa2 Pan-European Research Infrastructure on High Performance Computing; continuation of a large scale computational study on solvation of hydrophobic particles (140 kh of CPU time, AMD Opteron(tm) 2216 HE dual-core 2.4 GHz)

## PUBLICATIONS

### MS Thesis

DFT-calculations on  $Zn^{2+}$  within the zinc-finger-like domain of gag-protein p55, HIV, University of Vienna, April 1996.

### PhD Thesis

Development of a Novel Direct SCF Program for the Hartree Fock Treatment of Molecular Systems with Special Emphasis on Biomolecular Ligand Field and Reaction Field Problems, University of Vienna, September 1998.

1. MMDCG:Expansion Coefficients of Hermitian-Like Primitive Gaussians, S. Höfner, Program QCPE 678, *QCPE Bulletin*, **18**, 3, 27, Quantum Chemistry Program Exchange, (1998)
2. MDMFMT: Electron Repulsion Integrals, S. Höfner, Program QCPE 679, *QCPE Bulletin*, **18**, 3, 27, Quantum Chemistry Program Exchange, (1998)
3. Performance Analysis and Derived Parallelization Strategy for a SCF Program at the Hartree Fock Level, S. Höfner, O. Steinhauser and P. Zinterhof, *Lect. Notes Comp. Sci.*, **1557**, 163-172, (1999)
4. ERICHK: Check Program for Electron Repulsion Integrals, S. Höfner, Program QCPE 685, *QCPE Bulletin*, **19**, 2, Quantum Chemistry Program Exchange, (1999)
5. ELFCHK: Electric Field Integrals, S. Höfner, Program QCPE 686, *QCPE Bulletin*, **19**, 2, Quantum Chemistry Program Exchange, (1999)
6. Combined Hartree-Fock, Ligand Field and Multipolar Reaction Field Treatment of the Central Zinc Ion in HIV1 Zincfinger Peptide, S. Höfner and O. Steinhauser, *Book of Abstracts*, P.542, 5th World Congress of Theoretically Oriented Chemists, WATOC-99, (1999)

7. Performance Analysis, PVM and MPI Implementation of a DSCF Hartree Fock Program, S. Höfnger, O. Steinhauser and P. Zinterhof, *J. Comp. Inform. Technol.*, Special Issue on Parallel Numerics and Parallel Computing in Image Processing, Video Processing, and Multimedia, **8**, 1, 19-30, (2000)
8. Dielectric Relaxation in Proteins: A Continuum Electrostatics Model Incorporating Dielectric Heterogeneity of the Protein and Time-Dependent Charges, S. Höfnger and T. Simonson, *J. Comput. Chem.*, **22**, 3, 290-305, (2001)
9. Load Balancing for the Electronic Structure Program GREMLIN in a Very Heterogenous SSH-Connected WAN-Cluster of UNIX-Type Hosts, S. Höfnger, *Lect. Notes Comp. Sci.*, **2074**, 801-810, (2001)
10. POLCH: Polarization Charges, S. Höfnger, Program QCPE 805, Quantum Chemistry Program Exchange, (2001)
11. Making Use of Connolly's Molecular Surface Program in the Iso-Density Adapted Polarizable Continuum Model, S. Höfnger and O. Steinhauser, *J. Chem. Phys.*, **115**, 23, 10636-10646, (2001)
12. Method/Basis Set Dependence of the Traceless Quadrupole Moment Calculation for N<sub>2</sub>, CO<sub>2</sub>, SO<sub>2</sub>, HCl, CO, NH<sub>3</sub>, PH<sub>3</sub>, HF and H<sub>2</sub>O, S. Höfnger and M. Wendland, *Int. J. Quantum Chem.*, **86**, 2, 199-217, (2002)
13. Dynamic Load Equilibration for Cyclic Applications in Distributed Systems, S. Höfnger, *Lect. Notes Comp. Sci.*, **2330**, 963-971, (2002)
14. Opportunities and Challenges in Utilizing Application Specific Integrated Circuits in Drug Design, S. Höfnger, A. Berces, T. Narumi, T. Ebisuzaki, *SCI 2002 Proceedings*, 7th World Multiconference on Systemics, Cybernetics and Informatics, **16**, (2002)
15. Hardware Accelerated Molecular Dynamics of the Arabinose Binding Protein, S. Höfnger and A. Berces, *Book of Abstracts, PB317*, 6th World Congress of Theoretically Oriented Chemists, WATOC-02, (2002)
16. Automatic Runtime Load Balancing of Dedicated Applications in Heterogeneous Environments, S. Höfnger, *Lect. Notes Comp. Sci.*, **2474**, 62-69, (2002)
17. Parallel Global Optimization of High-Dimensional Problems, S. Höfnger, T. Schindler, A. Aszodi, *Lect. Notes Comp. Sci.*, **2474**, 148-155, (2002)
18. On the cavitation energy of water, S. Höfnger, and F. Zerbetto, *Chem-Eur. J.*, **9**, 2, 566-569, (2003)
19. Latency Reduction from Runtime-Interference to the Parallel Quantum Chemistry Program GREMLIN in Heterogeneous and Homogeneous Environments, S. Höfnger, *Future Gener. Comp. Sy.*, **19**, 5, 777-788, (2003)
20. The Free Energy of Nanobubbles in Organic Liquids, S. Höfnger and F. Zerbetto, *J. Phys. Chem. A*, **107**, 50, 11253-11257, (2003)
21. The costly process of creating a cavity in n-octanol, S. Höfnger and F. Zerbetto, *Theor. Chem. Acc.*, **112**, 4, 240-246, (2004)
22. What Size Cluster Equals a Dedicated Chip, S. Höfnger, *Lect. Notes Comp. Sci.*, **3241**, 397-404, (2004)
23. A Poisson-Boltzmann Solver running on the specialized computer chip MD-GRAPE-2: a case study on the effect of explicit consideration of counter ions, S. Höfnger, *Book of Abstracts, C11-5*, 7th Congress of the World Association of Theoretically Oriented Chemists, WATOC-05, 20, (2005)

24. The Collapse of Nanobubbles in Water,  
F. Lugli, S. Höfinger, F. Zerbetto, *J. Am. Chem. Soc.*, **127**, 22, 8020-8021, (2005)
25. Solving the Poisson Boltzmann Equation with the Specialized Computer Chip MD-GRAPE-2,  
S. Höfinger, *J. Comput. Chem.*, **26**, 11, 1148-1154, (2005)
26. Probing the Applicability of Polarizable Force-Field Molecular Dynamics for Parallel Architectures: a Comparison of Digital MPI with LAM-MPI and MPICH2,  
B. Almeida, R. Mahajan, D. Kranzlmüller, J. Volkert, S. Höfinger, *Lect. Notes Comp. Sci.*, **3666**, 433-440, (2005)
27. A new mechanistic model for Interleukin-4 receptor signaling across the lipid bilayer,  
T. Weidemann, S. Höfinger, M. Auer, *Eur. Biophys. J. Biophys.*, **34**, 6, 657, (2005)
28. Simple models for hydrophobic hydration,  
S. Höfinger, F. Zerbetto, *Chem. Soc. Rev.*, **34**, 12, 1012-1020, (2005) → **inside front cover**
29. A Very General Solvation Model for BioMolecular Simulation,  
S. Höfinger, *Publication Series of the John von Neumann Institute for Computing*, **34**, 87-90, (2006)
30. Large Scale Molecular Dynamics Simulations for the Derivation of Solvation Free Energies of Strongly Hydrophobic Molecules, R. Mahajan, D. Kranzlmüller, J. Volkert, S. Höfinger, *Publication Series of the John von Neumann Institute for Computing*, **34**, 173-176, (2006)
31. The Influence of Molecular Surface Composition on the Outcome of Poisson Boltzmann Calculations Performed to Obtain Solvation Free Energies,  
P. Kar, Y. Wei, U.H.E. Hansmann, S. Höfinger, *Publication Series of the John von Neumann Institute for Computing*, **34**, 161-164, (2006)
32. A critical  $\beta$ 6- $\beta$ 7 loop in the Pleckstrin Homology domain of ceramide kinase,  
P. Rovina, M. Jaritz, S. Höfinger, C. Graf, P. Dévay, A. Billich, T. Baumruker, F. Bornancin, *Biochem. J.*, **400**, 255-265, (2006)
33. Assessment and Tuning of a Poisson Boltzmann Program that Utilizes the Specialized Computer Chip MD-GRAPE-2 and Analysis of the Effect of Counter Ions,  
S. Höfinger, *Modelling Molecular Structure and Reactivity in Biological Systems*, RSC Publishing, ISBN 0 85404 668 2, 151-162, (2006)
34. Computational Assessment of the Entropy of Solvation of Small-Sized Hydrophobic Entities,  
R. Mahajan, D. Kranzlmüller, J. Volkert, U.H.E. Hansmann, S. Höfinger, *Phys. Chem. Chem. Phys.*, **8**, 5515-5521, (2006)
35. Beyond dimerization: a membrane-dependent activation model for Interleukin-4 receptor mediated signalling,  
T. Weidemann, S. Höfinger, K. Müller, M. Auer, *J. Mol. Biol.*, **366**, 1365-1373, (2007) → **see comments by the Faculty of 1000**
36. Parallel Tempering Molecular Dynamics Folding Simulation of a Signal Peptide in Explicit Water,  
S. Höfinger, B. Almeida, U.H.E. Hansmann, *Proteins*, **68**, 662-669, (2007)
37. Comparing Semi-Empirical versus Classic Charge Assignments in BioMolecules and their Effect on Electrostatic Potentials,  
P. Kar, M. Seel, U.H.E. Hansmann, S. Höfinger, *Publication Series of the John von Neumann Institute for Computing*, **36**, 155-157, (2007)
38. Algorithmic Refinements to an Enhanced Poisson-Boltzmann Approach used in BioMolecular Simulation,  
P. Kar, M. Seel, U.H.E. Hansmann, S. Höfinger, *Publication Series of the John von Neumann Institute for Computing*, **36**, 173-176, (2007)

39. Dispersion Terms and Analysis of Size- and Charge-Dependence in an Enhanced Poisson-Boltzmann Approach,  
P. Kar, M. Seel, U.H.E. Hansmann, S. Höfinger, *J. Phys. Chem. B*, **111**, 8910-8918, (2007)
40. Systematic Study of the Boundary Composition in Poisson Boltzmann Calculations,  
P. Kar, Y. Wei, U.H.E. Hansmann, S. Höfinger, *J. Comput. Chem.*, **28**, 2538-2544, (2007)
41. Detecting Secondary Bottlenecks in Parallel Quantum Chemistry Applications Using MPI,  
R. Mahajan, D. Kranzlmüller, J. Volkert, U.H.E. Hansmann, S. Höfinger, *Int. J. Mod. Phys. C.*, **19**, 1, 1-13, (2008)
42. Hydrophobicity — its Origin and an Important Example,  
S. Höfinger, M. Calvaresi, F. Lugli, F. Zerbetto, *Science and Supercomputing in Europe, HPC-EUROPA++ Report 2008*, edited by P. Alberigo, G. Erbacher, F. Garofalo, 230-236, (2008)
43. Signaling of IL4-R, a typical class I cytokine receptor: what defines the quiescent state ?  
T. Weidemann, S. Höfinger, M. Auer, *Handbook of Cell Signalling*, 2nd edition, edited by Ralph A. Bradshaw & Edward A. Dennis, chapter 47, 323-328, (2009)
44. Current Performance Gains from Utilizing the GPU or the ASIC MDGRAPE-3 within an Enhanced Poisson Boltzmann Approach,  
T. Narumi, K. Yasuoka, M. Taiji, S. Höfinger, *J. Comput. Chem.*, **30**, 14, 2351-2357, (2009)
45. Theoretical mimicry of biomembranes,  
P. Kar, M. Seel, T. Weidemann, S. Höfinger, *FEBS Lett.*, **583**, 12, 1909-1915, (2009)
46. Introducing Temperature Dependence in an Enhanced Poisson-Boltzmann Approach,  
S. Höfinger, F. Zerbetto, *Chem. Phys. Lett.*, **480**, 313-317, (2009)
47. Hydrophobic Hydration at Critical Length Scale — A HPC Endeavour,  
S. Höfinger, F. Zerbetto, *Proceedings, TAM 2009, Montpellier*, (2010) in press
48. Split Impressions from Large Scale Computational Analysis of Hydrophobic Phenomena Carried out on two Different HPC Architectures,  
S. Höfinger, F. Zerbetto, *HPC-EUROPA-2 Report 2009*, edited by P. Alberigo, G. Erbacher, F. Garofalo, (2010) in press
49. A RNA-based nanodevice recording temperature over time,  
S. Höfinger, F. Zerbetto, *Chem. Phys. Lett.*, **369**, 91-95, (2010)
50. Fast Calculation of Electrostatic Potentials on the GPU or the ASIC MD-GRAPPE-3,  
T. Narumi, K. Yasuoka, M. Taiji, F. Zerbetto, S. Höfinger, *Comput. J.*, (2010) in press
51. Focus on composition and interaction potential of single-pass transmembrane domains,  
R. Worch, C. Bökel, S. Höfinger, P. Schwille, T. Weidemann, *Proteomics*, (2010) in press

5 confidential Novartis internal reports  
several more articles in preparation