

# LIST OF PUBLICATIONS

STEFAN GOEDECKER

## Books

- S. Goedecker, A. Hoisie: "Performance Optimization of Numerically Intensive Codes", SIAM publishing company, Philadelphia, USA 2001 (ISBN 0-89871-484-2)
- S. Goedecker: "Wavelets and their application for the solution of partial differential equations", Presses Polytechniques Universitaires et Romandes, Lausanne, Switzerland 1998, (ISBN 2-88074-398-2)

## Papers (peer reviewed articles)

- M. Amsler, S. Alireza Ghasemi, S. Goedecker, A. Neelov and L. Genovese: Adsorption of small NaCl clusters on surfaces of silicon nanostructures *Nanotechnology* **20**, 00 (2009)
- Luigi Genovese, Matthieu Ospici, Thierry Deutsch, Jean-Francois Mhaut, Alexey Neelov and Stefan Goedecker: Density functional theory calculation on many-cores hybrid central processing unit-graphic processing unit architectures *J. Chem. Phys.* **131**, 034103 (2009)
- Shantanu Roy, Stefan Goedecker, Martin J. Field, Evgeni Penev: A minima-hopping study of all-atom protein folding and structure prediction, *J. Phys. Chem. B*, 2009, **113** (20), pp 73157321
- Sandro Schoenborn, Stefan Goedecker, Shantanu Roy and Artem Oganov: Evolutionary Algorithms and Minima Hopping for cluster structure prediction, *J. Chem. Phys.* **130** 144108 (2009)
- Pablo Pou, S. Alireza Ghasemi, Pavel Jelinek, Stefan Goedecker and Tom Lenosky: Structure and Stability of Semiconductor Tip Apexes for Atomic Force Microscopy, *Nanotechnology Journal* **20** 264015 (2009)
- Kuo Bao, Stefan Goedecker, Kenji Koga, Frederic Lancon, and Alexey Neelov: Structure of large gold clusters obtained by global optimization using the minima hopping method, *Phys. Rev. B* **79** 041405 (2009)
- Luigi Genovese, Alexey Neelov, Stefan Goedecker, Thierry Deutsch, Alireza Ghasemi, Oded Zilberberg, Anders Bergman, Mark Rayson and Reinhold Schneider: Daubechies wavelets as a basis set for density functional pseudopotential calculations: *J. Chem. Phys.* **129**, 014109 (2008)
- Alireza Ghasemi, Stefan Goedecker, Tom Lenosky, Hans Hug, Ernst Meier, Alexis Baratoff: Ubiquitous Mechanisms of Energy Dissipation in Noncontact Atomic Force Microscopy, *Phys. Rev. Lett.* **100**, 236106 (2008)

- Shantanu Roy, Stefan Goedecker and Vladimir Hellmann: A Bell-Evans-Polanyi principle for molecular dynamics trajectories and its implications for global optimization, *Phys. Rev. E* **77**, 056707 (2008)
- S. Alireza Ghasemi, Alexey Neelov, and Stefan Goedecker: A particle-particle, particle-density algorithm for the calculation of electrostatic interactions of particles with slablike geometry, *J. Chem. Phys.* **127**, 224102 (2007)
- Luigi Genovese, Thierry Deutsch, and Stefan Goedecker: Efficient and accurate three-dimensional Poisson solver for surface problems, *J. Chem. Phys.* **127**, 054704 (2007)
- Alexey Neelov, S. Alireza Ghasemi, and Stefan Goedecker: Particle-particle, particle-scaling function algorithm for electrostatic problems in free boundary conditions, *J. Chem. Phys.* **127**, 024109 (2007)
- Waldemar Hellmann, R. G. Hennig, Stefan Goedecker, C. J. Umrigar, Bernard Delley, and T. Lenosky: Questioning the existence of a well defined ground state for silicon clusters, *Phys. Rev. B* **75**, 085411 (2007)
- Luigi Genovese, Thierry Deutsch, Alexey Neelov, Stefan Goedecker and Gregory Beylkin: Efficient solution of Poisson's equation with free boundary conditions, *J. Chem. Phys.* **125**, 074105 (2006)
- A. I. Neelov and S. Goedecker: An efficient numerical quadrature for the calculation of the potential energy of wavefunctions expressed in the Daubechies wavelet basis, *J. of Comp. Phys.* **217**, 312-339 (2006)
- Stefan Goedecker, Waldemar Hellmann and Tom Lenosky: Global Minimum Determination of the Born-Oppenheimer Surface within Density Functional Theory, *Phys. Rev. Lett.* **95**, 055501 (2005)
- Stefan Goedecker: Minima hopping: An efficient search method for the global minimum of the potential energy surface of complex molecular systems, *J. Chem. Phys.* **120** 9911 (2004)
- Stefan Goedecker and Gustavo Scuseria: Linear Scaling Electronic structure methods in Physics and Chemistry, *Comp. in Sc. and Engin.* **5** 14 (2003)
- Stefan Goedecker, Mireille Boulet, Thierry Deutsch: An efficient 3-dim FFT for plane wave electronic structure calculations on massively parallel machines composed of multiprocessor nodes, *Comp. Phys. Commun.* **154** 105 (2003)
- Stefan Goedecker and Claire Chauvin: Combining multigrid and wavelet ideas to construct more efficient multiscale algorithms for the solution of Poisson's equation, *Journal of Theoretical and Computational Chemistry*, **2**, 483 (2003)
- Stefan Goedecker: Linear scaling methods for the solution of Schrödinger's equation, to appear in "Handbook of numerical analysis, special volume Computational chemistry, edited by PG Ciarlet and C. Le Bris, (North-Holland 2003)."

- S. Goedecker, X. Gonze: Electronic Structure and Vibrational Properties of Large Systems:  $O(N)$  Methods in *"handbook of materials science*, edited by L. Benett, (Elsevier, 2002)
- Stefan Goedecker: Optimization and Parallelization of a force field for silicon using OpenMP, *Comp. Phys. Comm.* **148** 124 (2002)
- Stefan Goedecker, Thierry Deutsch and Luc Billard: A fourfold coordinated point defect in silicon, *Phys. Rev. Lett.* **88**, 235501 (2002)
- G. Csanyi, S. Goedecker and T. Arias: Improved tensor product expansion for the two-particle density matrix, *Phys. Rev. A* **65**, 032510 (2002)
- Stefan Goedecker, Frédéric Lançon, Thierry Deutsch: Linear scaling relaxation of the atomic positions in nano structures, *Rapid Commun. in Phys. Rev. B* **64**, 161102-1 (2001)
- E. Koch and S. Goedecker: Locality properties and Wannier functions for interacting systems, *Sol. State Comm.*, **119** 105 (2001)
- S. Goedecker, C. Umrigar: Natural Orbital Functional Theory, in *"Many-electron densities and reduced density matrices*, edited by J. Cioslowski, (Kluwer Academic, Dordrecht, 2000)
- J. D. Kress, S. R. Bickham, L. A. Collins, B. L. Holian, S. Goedecker: Tight-binding Molecular Dynamics of Shock Waves in Methane, *Phys. Rev. Lett.* **83**, 3896 (1999)
- S. Goedecker:  $O(N)$  methods for electronic structure calculations, *Rev. of Mod. Phys.* **71**, 1085-1123, (1999)
- S. Goedecker, O. Ivanov: Hyper-sparsity of the density matrix in a wavelet representation, *Phys. Rev. B* **59**, 7270 (1999)
- J. Kress, S. Goedecker, A. Hoisie, H. Wassermann, O. Lubeck, L. Collins and B. Holian: Parallel  $O(N)$  Tight Binding Molecular Dynamics of Polyethylene and Compressed Methane, *Journal of Computer-Aided Materials Design*, **5**, 295 (1998)
- S. Goedecker: Decay properties of the finite temperature density matrix in metals, *Phys. Rev. B* **58**, 3501 (1998)
- C. Hartwigsen, S. Goedecker and J. Hutter: Relativistic separable dual-space Pseudopotentials from H to Rn, *Phys. Rev. B* **58**, 3641 (1998)
- S. Goedecker, C. Umrigar: Natural orbital functional for the many electron problem, *Phys. Rev. Lett.* **81**, 866 (1998)
- S. Goedecker, O. Ivanov: Solution of Multiscale Partial Differential Equations Using Wavelets, *Comp. in Phys*, **12**, 548 (Nov/Dec 1998)

- S. Goedecker, O. Ivanov: Linear Scaling solution of the classical Coulomb problem using wavelets, *Sol. State Comm.*, **105** 665 (1998)
- S. Goedecker and A. Hoisie: Scalable TB calculations for large polymer systems, Los Alamos National laboratory, unclassified report, LA-UR-97-1504 (1997)
- S. Goedecker, C. Umrigar: A critical assesment of the self-interaction corrected Local Density Functional method and its algorithmic implementation, *Phys. Rev. A* **55**, 1765 (1997)
- A. Hoisie and S. Goedecker: Scalable parallel electronic structure calculations on the IBM SP2, technical report CTC96TR254 , Cornell Theory Center, August 1996
- S. Goedecker: Fast radix 2,3,4 and 5 kernels for Fast Fourier Transformations on computers with overlapping multiply-add instructions, *SIAM Journal on Scientific Computing* **18**, 1605 (1997)
- S. Goedecker, M. Teter, J. Hutter: Separable dual space Gaussian Pseudopotentials, *Phys. Rev. B* **54**, 1703 (1996)
- S. Goedecker and M. Teter: Tight binding electronic structure calculations and tight binding molecular dynamics with localized orbitals, *Phys. Rev. B* **51**, 9455 (1995)
- S. Goedecker and L. Colombo: Tight binding molecular dynamics on parallel computers, technical report CTC94TR183, Cornell Theory Center, June 1994
- S. Goedecker and L. Colombo: An efficient linear scaling algorithm for tight binding molecular dynamics, *Phys. Rev. Lett* **73**, 122 (1994)
- S. Goedecker: Efficient iterative diagonalization of separable pseudopotential Hamiltonians, *Phil. Mag.* **70**, 305 (1994)
- S. Goedecker: Remark on algorithms to find roots of polynomials, *SIAM Journal on Scientific Computing*, **15**, 1059 (1994)
- S. Goedecker: An integral representation of the Fermi distribution and its applications in electronic structure calculations, *Phys. Rev. B* **48**, 17573 (1993)
- S. Goedecker: Low Complexity Algorithms for Density Functional Electronic Structure Calculations, *J. of Comp. Phys.* **118**, 261 (1995)
- S. Goedecker: Treatment of semicore states in the LAPW method, *Phys. Rev. B* **47** 9881 (1993)
- S. Goedecker: Rotating a three-dimensional array in optimal positions for vector processing: Case study for a three-dimensional Fast Fourier Transform, *Comp. Phys. Commun.* **76**, 294 (1993)
- S. Goedecker and K. Maschke: The operator approach in the LAPW method: Efficient electronic structure calculations including forces, *Phys. Rev. B* **45**, 1597 (1992)

- S. Goedecker and K. Maschke: Transferability of Pseudopotentials, Phys. Rev. A **45**, 88 (1992)
- S. Goedecker and K. Maschke: Comment on: Criterion for a good variational wave function, Phys. Rev. B **44**, 10365 (1991)
- S. Goedecker and K. Maschke: Alternative approach to first-principles pseudopotentials Phys. Rev. B **42**, 8858 (1990)
- S. Goedecker and K. Maschke: Fast iterative diagonalization of nonlocal pseudopotential Hamiltonians using the fast Fourier transformation, Phys. Rev. B **41**, 3230 (1990)
- S. Goedecker and R. Schwarz: Nonlinear recombination and diffusion in amorphous semiconductor films, H.P.A **61** 144 (1988)

## Seminars given at

- Max Planck Institute for Solid State Research, Stuttgart, Germany
- Technical University Munich, Munich, Germany
- Schottky Institute, Munich, Germany
- Technical University Bratislava, Bratislava, Czechoslovakia
- Cornell University, Ithaca, USA
- Naval Research Laboratory, Washington D.C., USA
- University of Illinois at Urbana-Champaign, Urbana-Champaign, USA
- University Mainz, Mainz, Germany
- Ciba-Geigy Limited, Basel, Switzerland
- Swiss Federal Institut of Technology (EPFL), Lausanne, Switzerland
- Kernforschungszentrum Jülich, Jülich, Germany
- IBM Central Research Lab. Europe, Rüschlikon, Switzerland
- Swiss National Supercomputing Center, Manoa, Switzerland
- College of William and Mary, Williamsburg, USA
- University of Montreal, Montreal, Canada
- Université Catholique, Louvain la Neuve, Belgium
- Los Alamos National Laboratory, Los Alamos, USA
- Cambridge University, Cambridge, England
- Oxford University, Oxford, England
- University of Edinburgh, Edinburgh, England
- Keele University, Keele, England
- University of Belfast, Belfast, England
- Eidgenössische Technische Hochschule (ETH), Zürich, Switzerland
- Beckmann Institut, Urbana-Champaign, USA
- Gesellschaft für Mathematik und Datenverarbeitung, St. Augustin, Germany
- Stuttgart University, Stuttgart, Germany

- Fritz-Haber Institut, Berlin, Germany
- Lawrence Berkeley National Laboratory, Berkeley, USA
- Rice University, Houston, USA
- Technical University Chemnitz, Germany
- University of California, Davis
- Ecole National supérieure, Lyon, France
- Queen's University, Kingston, Canada
- Max-Planck Institute, Dresden, Germany
- University of Bonn, Germany
- University of Zuerich, Switzerland
- University of Bochum, Germany
- National Institute of Materials Sciences, Tsukuba, Japan
- National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan
- Purdue University, West-Lafayette, USA
- Royal Institute of Technology, Stockholm, Sweden
- University of Vienna, Austria
- University of Erlangen, Germany

## Invited talks at major international conferences

- International Computational Materials Science Research Conference, West Virginia, 1995: "Tight Binding electronic structure calculations with linear scaling with respect to system size"
- European center for Atomic and Molecular Computations, Workshop "Linear-scaling methods in electronic-structure theory", Lyon 1995: "Tight binding electronic structure calculations and tight binding molecular dynamics based on a polynomial expansion of the finite temperature density matrix."
- European Total Energy workshop, Paris 1996: "Pseudopotentials with optimal properties for real space implementations"
- March meeting of the American Physical Society, St. Louis, 1996: "Electronic structure calculations using localized orbitals"
- US Electronic structure workshop, Minneapolis, 1996: "Electronic structure calculations using localized orbitals"
- European Center for Atomic and Molecular Computations, workshop "Going beyond the local density approximation in physics and chemistry", Lyon 1996: "A critical assesment of the self-interaction corrected Density Functional method"
- Supercomputing 1996, Pittsburgh, USA 1996: "Selfinteraction corrected density functional calculations on parallel computers"
- Supercomputer, Mannheim, Germany, 1997: "Tutorial on performance optimization on modern RISC computer architectures"
- International Conference on Computational Physics, Santa Cruz, USA, 1997: "Tutorial on performance optimization on modern RISC computer architectures"
- International Conference on Computational Physics, Granada, Spain, 1998: "The solution of multiscale differential equations using wavelets"
- Wavelets and Application Workshop, Locarno, Switzerland, 1998: "The solution of multiscale differential equations using wavelets"
- Ninth international workshop on computational materials science, electronic structure theory and simulations, Trieste, Italy, 1999: "Natural Orbital Functional Theory"
- European Center for Atomic and Molecular Computations, workshop "Recent developments in the theory of Wannier functions and other localized electronic wavefunctions", Lyon, June 1999, "Many body Wannier functions"
- SEMAT (Structure Electronique et Matériaux), Monastère de Mont-Sainte-Odile, October 1999, "Natural Orbital Functional Theory"

- GAMM workshop, Techniques for the solution of the Schrödinger equation, Leipzig, January 2000, "Wavelets for electronic structure calculations"
- March meeting of the American Physical Society, Minneapolis, March 2000: Tutorial on high performance computing in physics
- Psi\_k conference, Schwäbisch-Gmünd, 2000: "An overview over O(N) methods"
- SANSYMOC1, Strassbourg, March 2001: "The mathematical foundations of O(N) electronic structure methods"
- Spring meeting of the American Chemical Society, San Diego, April 2001: "The locality principle of chemistry and its reflection in O(N) methods for electronic structure"
- European Center for Atomic and Molecular Computations, workshop "Local orbitals and linear-scaling ab initio calculations" Lyon, September 2001: "Wavelets for electronic structure calculations"
- Workshop on modern aspects of many-electron theory, Bad Honnef, November 2001: "Recent developments in Natural Orbital Functional Theory"
- March meeting of the American Physical Society, Indianapolis, March 2002, "Localization properties of the density matrix and Wannier functions"
- IPAM meeting on linear scaling methods, Los Angeles, April 2002, "Achieving Linear Scaling in atomistic simulations"
- European Center for Atomic and Molecular Computations, workshop on Exchange Correlation Functionals: Assessment and Prospects, Lyon, June 2002: "Recent developments in Natural Orbital Functional Theory"
- European Center for Atomic and Molecular Computations, workshop on Open Source Software for Microscopic Calculations, Lyon, June 2002: "Performance optimization"
- Weierstrass Institute for Applied Analysis and Stochastics, workshop on Multiscale Problems in Quantum and Classical Mechanics, Averaging Techniques and Young Measures, September 2002: "The common concepts of Wavelets, Multigrid and Fast Multipole methods for the solution of Poisson's equation"
- Spring meeting of the American Chemical Society, New Orleans, March 2003: "Preconditioning iterative methods for electronic structure calculations"
- 33rd speedup workshop, Basel, March 2003: "Plane Wave Electronic Structure Calculations on Parallel Computers Composed of Multiprocessor Nodes"
- Total energy workshop, Januar 2004, Paris, "Global geometry optimization with minima hopping"
- Electronic structure conference, May 2004, Rutgers University: "Global geometry optimization with minima hopping"

- Computational Science Workshop, March 2005, Tsukuba Japan, "Linear scaling electronic structure calculations"
- Workshop Breaking complexity, Bad Honnef, Dec. 2005, "Wavelet basis sets for Schrödinger's equation"
- 3rd International ABINIT Developer Workshop, Liege Belgium, January 2007, "Wavelets for electronic structure calculations"
- Workshop, Classical and Quantum Approaches in Molecular Modeling, August 2007, Minneapolis, "Wavelets for electronic structure calculations"
- CECAM workshop, Linear-scaling ab initio calculations: applications and future directions, Lyon Sept. 2007, "Linear scaling in a wavelet basis"
- CECAM tutorial, High performance density functional theory : wavelets, order(N) scaling, parallelism , Lyon Nov. 2007, "How to use wavelets in electronic structure calculations"
- SIAM conference on mathematical problems in materials sciences, Philadelphia, May 2008: "The BigDFT wavelet based electronic structure package"
- Winter School Multiscale Simulation Methods in Molecular Sciences Jülich, March 2009: "Wavelets and Their Application for the Solution of Poissons and Schrdingers Equation"
- Workshop on Structure Prediction of Clusters, London, September 2009: "Global geometry optimization with the minima hopping method"
- Nanoelectronics meeting, Canadian Institute for Advanced Research, Quebec City, Canada, November 2009: "Structure prediction on the nano scale"

## Teaching activities

- Semester course "Computational Physics": Numerical methods from all fields of condensed matter physics such as Molecular dynamics, Monte Carlo methods, fast treatment of  $1/r$  potentials
- Semester course "Electronic structure": Hartree Fock, Configuration Interaction, Coupled Cluster, Many Body perturbation Theory, Density functional Theory, Quantum Monte Carlo
- Semester course "Statistical physics for nanosciences": Basic principles of statistical physics and their application to problems in chemistry, biology and physics.
- Block course "Atomistic simulations": Elementary simulation methods for structure determination and dynamics
- Block course "Density functional theory": Introduction to Density functional Theory
- Numerous tutorials at conferences and workshops on topics such as High performance computing, Wavelets, Density functional theory, iterative methods