

Andreas Pedersen

November 2nd 1978
Danish Citizenship
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Employment

Research Scientist, Science Institute (2010-)
University of Iceland, IS

Post Doctoral Fellow, Instituto de Matemática Interdisciplinar (2009-2010)
Project Title: A computational study of UV radiation on interstellar dust
Universidad Complutense de Madrid, ES

Post Doctoral Fellow, School of Science and Engineering (2008-2009)
Project Title: Investigation of Basic Properties of Vacuum Microelectronic Devices
Reykjavík University, IS

IT-supporter, (2002-2003)
Forskningssentret for Skov & Landskab, DK

Educational Background

Doctor of Philosophy, Computational Chemistry (2008)
Project Title: Long Time Scale Simulations of Materials using Distributed Computing
University of Iceland, IS
Supervisor Prof. Hannes Jónsson; Department of Chemistry, HI, IS
Co-supervisor Dr. Jakob Schiøtz; Department of Physics, DTU, DK

Master of Engineering, Applied Physics (2004)
Project Title: Temperature Accelerated Dynamics
Technical University of Denmark, DK
Supervisor Dr. Jakob Schiøtz; Department of Physics, DTU, DK

Bachelor of Engineering, Applied Physics (2002)
Project Title: Degassing through an interface
Technical University of Denmark, DK
Supervisor Dr. René Fléron; The Microelectronic Center, DTU, DK

Extended Collaboration Visits

Prof. G. Henkelman; Department of Chemistry and Biochemistry, UT, USA (4 months)
Prof. H Jónsson; Department of Chemistry, UW, USA (3 months)
Prof. L. Pizzagalli; PHYMAT, University of Poitiers, FR (2 months)
Dr. J. Schiøtz; Department of Physics, DTU, DK (2 months)
Prof. Arthur Voter; T-12, LANL, USA (1 month)

Research Interests

Scientific Computing; Cloud, Distributed and Parallel Computing; Methodology and Algorithm Development; Optimization; Visualization; Complex Systems

Publications

- Theoretical study of kinks on screw dislocation in silicon*
L. Pizzagalli, A. Pedersen, A. Arnaldsson, H. Jónsson and P. Beauchamp
Physical Review B; 77, 064106 (2008)
- Finding mechanism of transitions in complex systems: Formation and migration of dislocation kinks in a silicon crystal*
A. Pedersen, L. Pizzagalli and H. Jónsson
Journal of Physics: Condensed Matter; 21, 084210 (2009)
- Simulations of Hydrogen Diffusion at Grain Boundaries in Aluminum*
A. Pedersen and H. Jónsson
Acta Material; 57, 4036-4045 (2009)
- Long Time Scale Simulation of a Grain Boundary in Copper*
A. Pedersen, G. Henkelman, J. Schiøtz and H. Jónsson
New Journal of Physics; 11, 073034 (2009)
- Distributed Implementation of the Adaptive Kinetic Monte Carlo Method*
A. Pedersen and H. Jónsson
Mathematics and Computers in Simulation; 80, 1487 (2010)
- Space-charge modulation in vacuum microdiodes at THz frequencies*
A. Pedersen, A. Manolescu and Á. Valfells
Physical Review Letters; 104, 175002 (2010)
- Efficient sampling of saddle points with the minimum mode following method*
A. Pedersen, S. F. Hafstein and H. Jónsson
SIAM Journal on Scientific Computing 32, 633 (2011)

Accepted Publications

- The charging profile of dust grains in the environment of Young Stellar Objects*
A. Pedersen and A. I. Gomez de Castro
The Astrophysical Journal
- Simulated Annealing with Coarse Graining and Distributed Computing*
A. Pedersen, J. C. Berthet and H. Jónsson
Lecture Notes in Computer Science

Submitted Publications

- Coarse graining Monte Carlo algorithm*
J. C. Berthet, A. Pedersen and H. Jónsson
New Journal of Physics

Selected Oral Presentations

- Adaptive kinetic Monte Carlo simulations of H-diffusion in metal grain Boundaries*
Invited, Workshop on Multiscale Modeling;
Leuven, Belgium (July 2008)
- Atomistic dynamics using distributed and grid computing*
Invited, PARA2010 10th conference on State of the Art in Scientific and Parallel Computing;
Reykjavik, Iceland (June 2010)
- Atomistic dynamics using distributed and grid computing*
Invited, Los Alamos National Laboratory;
Los Alamos, USA (December 2010)
- Atomistic dynamics using distributed computing*
Invited, China University of Geosciences;
Wuhan, China (April 2011)

Funding Obtained

1. *The Icelandic Research Fund administered by RANNIS, 12.540.000 Isk (2010-2012)*
2. *The University of Iceland Research fund 700.000 Iskr (2011)*
3. *Awarded with NILS mobility grant from UCM-EEA Abel, 42.000 € (2009)*
4. *Awarded with travel grant from Otto Mønsted's fund, 7.000 Dkr (2003)*

Teaching Experience

TA Physical Chemistry 2, University of Iceland, IS
TA Physical Chemistry 3, University of Iceland, IS
TA Physical Chemistry 5, University of Iceland, IS
TA Basic Laboratory Work, DTU, DK
TA Chemistry, Thermodynamics and Material Science, DTU, DK

Refereeing Experience

Central European Journal of Physics, Versita (2010)
Journal of Physics and Chemistry of Solids , Elsevier (2009)
Surface and Interface Analysis, Wiley (2009)

Other

Transferred the distributed computer program EON, which was written during my Ph.D. studies, to Prof. Graeme Henkelman's research group at UT, Austin, USA and to Prof Hansong Chen's research group at CUG, Wuhan, China. The program is capable of using distributed public computers as the main computational resource rather than relying on a dedicated super-computer.

Developed and implemented software for high fidelity simulations of electron as a Post Doc at Universidad Complutense de Madrid and Reykjavík University. Plans at Reykjavík University are to evolve this code into a second generation.