David J. Schmidt

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OBJECTIVE A challenging and versatile position with special interests in quantitative and algorithmic programming, modeling, and simulations.

COMPUTER SKILLS *Languages & Software:* Linux C/C++, distributed/shared memory/hybrid Parallel Programming and multithreading, Windows C/C++/C#, Java Script, PHP, SQL, ASP.net, Matlab and Simulink, FORTRAN, Pascal, CSH, Bash, Assembly, LaTex. *Micro-Controller/Embedded Systems:* PIC, FPGA.

MODELING & SIMULATIONS *Simulation Methods:* Monte Carlo and Molecular Dynamics. *Modeling Methods:* Cluster Expansions, Least Squares/Cross Validation Fitting, Steepest Descent, Genetic Algorithm, Adaptive Filters, Elementary Neural Networks. *Quantum Mechanics Software:* Density Functional Theory (DFT) using VASP, Hartree-Fock using Gaussian.

EDUCATION

Doctorate of Philosophy, Chemical and Biomolecular Engineering, 3.53 GPA
University of Notre Dame, Notre Dame, IN January 2013
Concentration: Coverage Effects Simulations and Modeling

Bachelor of Science, Electrical Engineering and Chemistry, 3.6 GPA
California State Polytechnic University, Pomona, June 2007
Concentrations: Digital Signal Processing and Molecular Modeling

EXPERIENCE

Graduate Student - Adsorbate Coverage Effects Modeler August 2007-January 2013
University of Notre Dame, Notre Dame, IN. 46556

- Supervised Undergraduate Research and Senior Project of Martin Beres.
- TA for transport, advanced thermo, process control, and into to chem eng.
- Performed quantum mechanical density functional theory (DFT) with VASP.
- Fit cluster expansions to DFT results using cross validation for optimization.
- Wrote Monte Carlo code in Linux C/C++ with OMP and MPI parallelization.

C# Programmer March-August 2007
Eckersall, LLC, Chino, CA. 91710

- Programmed GIS websites for cell phones and desktops.
- Worked with C# in the .NET Framework with MS-SQL and with Coldfusion.

Math Tutor/Facilitator September 2003-December 2006
Mathematics and Science Help (MaSH) Center,
California State Polytechnic University, Pomona, CA. 91768

- Tutored mathematics from remedial to multivariate calculus, differential equations, Laplace and Fourier transforms, statistics, and physics.
- Facilitated remedial math lab classes.

Quality Control Engineer Intern June-December 2004
San Onofre Nuclear Generating Station (SONGS),
Southern California Edison, San Onofre, CA

- Inspected/tested materials to assure specification compliance.
- Materials tested included oil, grease, screws, nuts, bolts, breakers, thermistors, transistors, etc.

HONORS, & AWARDS

Tau Beta Pi (TBP) Engineering Honor Society, Initiated 2005
- Adviser, ING Chapter 2009-2012
- Prepared Successful Bid for 2011 National Convention, Nov. 2009
- President, CAN Chapter 2006-07

National Science Foundation Grant CBET07-31020
Cum Laude, Cal Poly Pomona 2007
Eta Kappa Nu (HKN) Electrical Engineering Honor Society, Initiated 2006
Meritorious Award for Mathematical Contest in Modeling (MCM) 2006
10+ Putnam Math Competition 2000, 2003, 2004 (median score is 1 or 2)

SOCIAL ACTIVITIES

Volunteered for Habitat for Humanity 2006-2010
Planted Rain Garden in South Bend Spring 2011

PUBLICATIONS

"Performance of Cluster Expansions for Coverage-Dependent Adsorption of Atomic Oxygen on Pt(111)," D Schmidt, W Chen, C Wolverton, W Schneider, Journal of Chemical Theory and Computation, December 9, 2011.

"Accurate coverage-dependence incorporated into first-principles kinetic models: Catalytic NO oxidation on Pt (111)," C Wu, D Schmidt, C Wolverton, and W Schneider, Journal of Catalysis, November 26, 2011.

"Ordering and Oxygen Adsorption in Au-Pt/Pt (111) Surface Alloys," W Chen, D Schmidt, C Wolverton, and W Schneider, Journal of Physical Chemistry C, Published August 8, 2011.

"First-Principles Cluster Expansion Study o Missing-Row Reconstructions of FCC (110) Surfaces," W Chen, D Schmidt, C Wolverton, and W. Schneider, Physical Review B, Published February 14, 2011.

"Intermediates and Spectators in O_2 Dissociation at the RuO_2 (110) Surface," H Wang, W Schneider, and D Schmidt, Journal of Physical Chemistry C, Published July 31, 2009.

CONFERENCE PRESENTATIONS

"Cluster Expansions of Dissociative Oxygen Adsorption on Metal (111) Surfaces: A Separation of Electronic and Strain Effects," Midwest Thermodynamics and Statistical Mechanics Conference, May 2012.

"Cluster Expansions Based Modeling of the Coverage Dependence of Adsorbate Binding at a Metal Surface," AICHE Annual Conference, November 2010.

"Cluster Expansions Applied to Adsorbate Ordering on Surfaces," Midwest Thermodynamics and Statistical Mechanics Conference, June 2010.

POSTER PRESENTATIONS

"Coverage Dependent Kinetic Modeling of Dissociative Oxygen Adsorption and NO Oxidation on Metal (111) Surfaces," Chicago Catalysis Conference, May 2012.

"Cluster Expansion Based Modeling of the Coverage Dependence of Adsorbate Binding at a Metal Surface," Chicago Catalysis Conference, May 2010.

"Cluster Expansion Based Modeling of the Coverage Dependence of Adsorbate Binding at a Metal Surface," AICHE, November 2009.