Max J. Hoffmann

892 Roble Ave
Menlo Park, CA 94025, USA
+1 650 521 7187
mjhoffmann@gmail.com
mhoffman.github.io

Work Experience

11/01/2014-present *Post-doctoral researcher*, Stanford University, Chemical Engineering Department
Prof. Dr. Jens Nørskov, Dr. Thomas Bligaard
- *model development for adsorbate-adsorbate interactions*
- *software development for advanced kinetic modeling*
- *first-principles computer simulations and data analysis*
- *project guidance for master students*

01/08/2014-30/10/2014 *Post-doctoral researcher*, TU Munich, Chair of Theoretical Chemistry
Prof. Dr. Karsten Reuter

Education

01/10/2010-31/07/2014 Ph.D. in Theoretical and Computational Chemistry, *summa cum laude*
Technische University Munich – Chair of Theoretical Chemistry
"*First-principles Multi-scale Simulations of Dynamic Catalyst Surfaces CO Oxidation from Palladium surface oxide to Palladium metal*"
advisor: Prof. Dr. Karsten Reuter
- *large-scale electronic structure calculations, multi-scale modeling*
- *method development, scientific software development*
- *supervision of bachelor thesis, 2nd level computer support*

01/04/2005-30/09/2010 Diploma, Physics, 1.0 with distinction (1.0-4.0, 1.0 best)
Free University Berlin
- *minor in Computer Science*
- *specialization in theoretical surface physics, condensed matter, and density functional theory*

09/01/2009-06/30/2010 Fritz-Haber-Institut der Max-Planck-Gesellschaft
Diploma Thesis supervisors: Prof. Dr. Karsten Reuter, Prof. Dr. Matthias Scheffler
09/01/2008-06/30/2009 University of California at Santa Barbara, UCSB
exchange year, independent research with Prof. Dr. Horia Metiu

15/07/1997-30/06/2004 Abitur, grade 1.6 (1.0-4.0, 1.0 best)
Paul-Natorp-Gymnasium (High School) Berlin
09/01/2001-06/30/2002 Gettysburg Area High School Gettysburg, PA, US
US High School Diploma

Scholarships & Awards

2013 Travel grant, Gordon Conference, *Chemical Reactions at Surfaces*, Diablerets, CH

2008 Freie Universität Berlin Direct Exchange Program
Participation in UC EAP program and one year of tuition at UC Santa Barbara

2005 Jugend Forscht (science fair), 1st place in Berlin competition

2001 Rotary Youth Exchange Scholarship

Skills and Technologies

Languages Python (7 years), Fortran (3 years), C (2 years), HTML, CSS, JavaScript, LaTeX, XML.

Tools Quantum Espresso, CASTEP, ASE, f2py, pygtk, Django, Lucene, Elasticsearch, jQuery, git, vim, bash, matplotlib, numpy, scipy, pandas, sklearn.

Other Linux system administration, Linux Professional Institute Certified (LPIC 1)
Extended software development experience: unit testing, assertions, version control.

Projects kmos (open source kinetic Monte Carlo modeling framework).

Languages

German (*native*)

English (*fluent*, U.S. High School Diploma, TOEFL iBT score 114/120)

Portuguese (*basic*)

Teaching Experience

Winter 2013 Tutor for Software Carpentry boot camp

Winter 2012 Methods of Theoretical Chemistry and Spectroscopy (Computer lab)

Sep 2011 Hands-on course for industry researchers on lattice kinetic Monte Carlo

Summer 2011 Math for Chemists II

Winter 2010 Methods of Theoretical Chemistry and Spectroscopy (Computer lab)

Publications

[1] Sebastian Matera, Sara Blomberg, Max Hoffmann, Johan Zetterberg, Johan Gustafson, Edvin Lundgren, and Karsten Reuter. Evidence for the active phase of heterogeneous catalysts through in situ reaction product imaging and multiscale modeling. *ACS Catalysis*, 2015.

[2] Andrew J. Medford, Chuan Shi, Max J. Hoffmann, Adam C. Lausche, Sean R. Fitzgibbon, Thomas Bligaard, and Jens K. Nørskov. Catmap: A software package for descriptor-based microkinetic mapping of catalytic trends. *Catalysis Letters*, 145(3):794–807, 2015.

[3] Max Hoffmann, Matthias Scheffler, and Karsten Reuter. Multi-lattice kinetic monte carlo simulations from first-principles: Reduction of the pd(100) surface oxide by CO. *ACS Catal.*, 5:1199–1209, 2015.

[4] Max J. Hoffmann, Sebastian Matera, and Karsten Reuter. kmos: A lattice kinetic monte carlo framework. *Computer Physics Communications*, 185(7):2138–2150, 2014.

[5] Max J. Hoffmann and Karsten Reuter. Co oxidation on pd(100) versus pdo(101)-$(\sqrt{5}\times\sqrt{5})r27^{\circ}$: First-principles kinetic phase diagrams and bistability conditions. *Topics in Catalysis*, 57(1-4):159–170, 2014.

[6] S. Blomberg, Max J. Hoffmann, J. Gustafson, N. M. Martin, R. Fernandes, A. Borg, Z. Liu, R. Chang, S. Matera, K. Reuter, and E. Lundgren. In situ X-Ray Photoelectron Spectroscopy of Model Catalysts: At the Edge of the Gap. *Physical Review Letters*, 110:117601–117606, 2013.

Conferences

[1] Bistability during CO oxidation at Pd(100): Atomistic origin from first-principles kinetic Monte Carlo simulations. In *Operando Research in Catalysis*, Leiden (NL), June 2013.

[2] Bistability during CO oxidation at Pd(100): Atomistic origin from first-principles kinetic Monte Carlo simulations. In *Gordon Research Conference Chemical Reaction at Surfaces*, Les Diablerets (CH), April 2013.

[3] Bistability during CO oxidation at Pd(100): Atomistic origin from first-principles kinetic Monte Carlo simulations. In *DPG Spring Meeting*, Regensburg, March 2013.

[4] Multi-lattice Monte Carlo Simulations of Substrate Morphological Transitions in CO Oxidation at Pd(100), *Poster*. In *ICC-15*, Munich, July 2012.

[5] Multi-lattice approach to first-principles kinetic monte carlo simulations: Application to catalytic CO oxidation at pd(100), *Talk*. In *APS March Meeting*, Boston, March 2012.

[6] Multi-lattice approach for first-principles kinetic Monte Carlo simulations on Pd(100), *Talk*. In *CRC Workshop with Northwestern University*, Garching, May 2011.

[7] Multi-Lattice Kinetic Monte Carlo Simulations of Substrate Morphological Transitions in CO Oxidation at Pd(100), *Poster*. In *16th Meeting of the Fachbeirat*, Fritz-Haber-Institut der Max-Planck-Gesellschaft, November 2011.