

Andreas Heyden

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Professional Preparation

<i>Institution</i>	<i>Major / Area</i>	<i>Degree & Year</i>
Hamburg University of Technology	Chemical Engineering	Diplom: 2000
Hamburg University of Technology	Chemical Engineering	Ph.D.: 2005
University of Minnesota	Theoretical Chemistry	Postdoc: 2006-2007

Appointments

2007 – present	Assistant Professor	Dept. of Chem. Eng., University of South Carolina
2007 – present	Assistant Professor	NanoCenter, University of South Carolina

Honor, Awards & Distinctions

Minnesota Supercomputing Institute Research Scholarship and Travel Grants	2006-2007
Council for the Lindau Nobel Laureate Meetings Participation Award	2006
Karl H. Ditze Award (leading Ph.D. thesis at the Hamburg University of Technology)	2006
Ewald Wicke Foundation Travel Grant	2005
Bayer AG Mentoring Program Membership	2000-2001
Charitable Trust of the German Industry Study Grant	1997-2000
German Academic Exchange Service Study Grant (to study at UC Berkeley)	1998-1999

Publications

Five most closely relevant to proposed project

Heyden, A., Lin, H., Truhlar, D. G., Adaptive partitioning in combined quantum mechanical and molecular mechanical calculations of potential energy functions for multiscale simulations. *J. Phys. Chem. B* **111**, 2231-2241 (2007).

Hansen, N., Heyden, A., Bell, A. T., Keil, F. J., Microkinetic modeling of nitrous oxide decomposition on binuclear oxygen bridged iron sites in Fe-ZSM-5. *J. Catal.* **248**, 213-225 (2007).

Hansen, N., Heyden, A., Bell, A. T., Keil, F. J., A reaction mechanism for the nitrous oxide decomposition on binuclear oxygen bridged iron sites in Fe-ZSM-5. *J. Phys. Chem. C* **111**, 2092-2101 (2007).

Heyden, A., Hansen, N., Bell, A. T., Keil, F. J., Nitrous oxide decomposition over Fe-ZSM-5 in the presence of nitric oxide: A comprehensive DFT study. *J. Phys. Chem. B* **110**, 17096-17114 (2006).

Heyden, A., Bell, A. T., Keil, F. J., Efficient methods for finding transition states in chemical reactions: Comparison of modified dimer method and partitioned rational function optimization method. *J. Chem. Phys.* **123**, 224101-14 (2005).

Five other significant publications

Iron, M. A., Heyden, A., Staszewska, G., Truhlar, D. G., Tight binding configuration interaction (TBCI): A non-iterative approach to incorporating electrostatics into tight binding. *J. Chem. Theory Comp.* **4**, 804-818 (2008).

Heyden, A., Truhlar, D. G., A conservative algorithm for an adaptive change of resolution in mixed atomistic / coarse-grained multiscale simulations. *J. Chem. Theory Comp.* **4**, 217-221 (2008).

Heyden, A., Bell, A. T., Keil, F. J., Kinetic modeling of nitrous oxide decomposition over Fe-ZSM-5 based on parameters obtained from first-principles calculations. *J. Catal.* **233**, 26-35 (2005).

Heyden, A., Peters, B., Bell, A. T., Keil, F. J., Comprehensive DFT study of nitrous oxide decomposition over Fe-ZSM-5. *J. Phys. Chem. B* **109**, 1857-1873 (2005).

Peters, B., Heyden, A., Bell, A. T., Chakraborty, A., A growing string method for determining transition states: Comparison to the nudged elastic band and string methods. *J. Chem. Phys.* **120**, 7877-7886 (2004).

Synergistic Activities

Developed highly efficient algorithms for finding transition states on high-dimensional potential energy surfaces. These algorithms are available upon request and have been implemented into Q-Chem, ChemShell, TURBOMOLE, and VASP, four widely distributed electronic structure program packages.

Collaborators & Other Affiliations

Prof. Arup K. Chakraborty (MIT), Dr. Tina Düren (University of Edinburgh, UK), Dr. Mark A. Iron (Weizmann Institute of Science, Israel), Prof. Hai Lin (University of Colorado – Denver), Prof. Baron Peters (University of California – Santa Barbara), Prof. Nigel Seaton (University of Edinburgh, UK)

Graduate Advisors and Postdoctoral Sponsor

Ph.D. Advisors	Prof. Frerich J. Keil, Hamburg University of Technology, Germany Prof. Alexis T. Bell, University of California, Berkeley, USA
Postdoctoral Advisor	Prof. Donald G. Truhlar, University of Minnesota, USA

Thesis Advisor and Postgraduate-Scholar Sponsor

<u>Postdoctoral Scholars</u>	<u>Graduate Students</u>	<u>Undergraduate Students (UG thesis)</u>
Salai Cheettu Ammal	Luay Hammami	George Hearn
Jong Hyuk Park	Suwit Suthirakun	