ANDREAS HEYDEN

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EDUCATION

Hamburg University of Technology Hamburg, Germany

Ph. D. in Chemical Engineering, December 2005
Thesis: "Theoretical investigation of the nitrous oxide decomposition over iron zeolite catalysts"
Advisor: Professor Frerich J. Keil
Co-Advisor: Professor Alexis T. Bell Grade: "with distinction"

Diplom in Chemical Engineering, December 2000 (undergraduate degree)
Thesis: "Transition from molecular simulation of adsorption and diffusion to process simulation of a PSA module"
Advisor: Professor Günter Gruhn
Co-Advisor: Professor Frerich J. Keil Grade: "with distinction" (1.1)

Vordiplom in Chemical Engineering, November 1997 (intermediate undergraduate degree)
Grade: "very good" (1.1)

University of California Berkeley Berkeley, California

Visiting scholar in the Department of Chemical Engineering, August – December 2001,
August – December 2002, August 2003 – March 2004
- Conducted research on Ph. D. thesis under Professor Alexis T. Bell. Attended various theoretical chemistry graduate classes.

Graduate exchange student in Chemical Engineering, August 1998 – May 1999

University of Edinburgh Edinburgh, UK

Visiting scholar in the Department of Chemical Engineering, June – September 2000
- Conducted research on Diploma thesis under Professor Nigel Seaton.

AWARDS

- *Minnesota Supercomputing Institute Research Scholarship*; Postdoctoral Fellowship, Academic year 2006 – 2007
- *Council for the Lindau Nobel Laureate Meetings Participation Award*; participant of the 18th Meeting of Nobel Prize Winners in Chemistry, Lindau, Germany; June 2006
- *Karl H. Ditze Award*; leading Ph. D. thesis at the Hamburg University of Technology, Academic year 2005 – 2006

- *Minnesota Supercomputing Institute Travel Grants*; AIChE 2006 annual meeting, FOMMS 2006 meeting
- *Ewald Wicke Foundation Travel Grant*; AIChE 2005 annual meeting
- *Bayer AG Mentoring Program Membership*, April 2000 – May 2001
- *Charitable Trust of the German Industry Study Grant*, May 1997 – December 2000
- *German Academic Exchange Service Study Grant*, Academic year 1998 – 1999

PROFESSIONAL EXPERIENCE

University of South Carolina Columbia Campus, South Carolina
Department of Chemical Engineering
Assistant Professor *August 16, 2007 – present*
Research areas: Computational nanomaterial science and catalysis – Multiscale modeling

- Study of the structure-performance relationship of systems relevant to catalysis and energy production/storage.
- Study of the effect of alloying and catalyst support on the structure, surface composition, and catalytic activity of supported metal clusters and nanoparticles.
- Development of novel multi-scale modeling strategies and their application to hard and soft matter systems.

University of Minnesota Twin Cities Campus, Minnesota
Department of Chemistry
Postdoctoral Fellow with Prof. Donald G. Truhlar
Nanomaterials subgroup *January 1, 2006 – August 1, 2007*

- Developed an adaptive partitioning method for combining multilevel methods such as QM/MM methods, with sampling schemes. Unlike previous QM/MM simulation algorithms, the method allows for the accurate study of processes in solution or the coupling of reaction to diffusion.
- Developed a conservative algorithm for an on-the-fly change of resolution in mixed atomistic / coarse-grained multiscale simulations.

Hamburg University of Technology Hamburg, Germany
Department of Chemical Engineering
Graduate Student Researcher with Prof. Frerich J. Keil and
Prof. Alexis T. Bell (UC Berkeley) *January 1, 2001 – December 31, 2005*

- Identified the active site and reaction mechanism of the N_2O decomposition over iron zeolite catalysts – a catalytic system relevant for the reduction of greenhouse gas emissions from nitric and adipic acid plants.
- Gained significant insights into the nature of the catalytically active sites at different temperatures and the effects of species such as water and nitric oxide that have eluded experimentalists.
- Developed highly efficient algorithms for finding transition states on high-dimensional potential energy surfaces. Helped to integrate the methods into the new version of Q-Chem 3.0 and ChemShell and the next release of TURBOMOLE and VASP, four widely distributed quantum chemistry program packages.

Undergraduate Student Researcher with Prof. Günter Gruhn *May – November 2000*

- Developed a configurational-biased Monte Carlo module for a Monte Carlo program and extended a molecular dynamics program to study molecules with internal constraints. Applied the programs to the study of adsorption and diffusion properties of small alkanes in multi-walled carbon nanotubes.
- Modeled the performance of a pressure swing adsorption module based on carbon nanotubes.

Undergraduate Student Researcher with Prof. Frerich J. Keil *April – July 1998*

- Conducted experimental studies for the determination of a reaction rate equation for the methane combustion on a palladium catalyst.

Bayer AG Leverkusen, Germany
External Consultant for Bayer Technology Services *January 1 – December 31, 2001*

- Developed computer programs to predict the solubility of chemical compounds in pharmaceutically relevant solvents. Advised on multi-component solubility problems.

Engineering Intern at Bayer Technology Services *August – November 1999*

- Developed programs to predict the affinity between macromolecules and solvent molecules to determine capsule material for aroma and drug substances. Conducted solubility experiments and improved a model for a stream dryer.

TEACHING EXPERIENCE

University of South Carolina Columbia, South Carolina
Research group members

Postdoctoral Associates

- Jong Hyuk Park
- Salai Cheettu Ammal

Graduate Students

- Hongliu Liu

Undergraduate Students

- George Hearn

Classes taught as professor

- ECHE 730: Chemical reactor design: Chemical engineering graduate class in chemical kinetics and reactor design, Fall 2007

Hamburg University of Technology Hamburg, Germany
Graduate Student Instructor

- Supervised one Master's thesis, two diploma theses, and five undergraduate research projects, 2001 – 2004
- Supervised four lab courses in chemical reaction engineering, Spring 2001 – 2004
- Presented tutorials in linear algebra, Academic year 2001 – 2002
- Supervised students in two process design courses, Spring 2001 and 2002

Refugee House Hamburg, Germany
Volunteer Instructor

- Taught African refugees calculus, German, and MS Office, 2001 – 2003

ADDITIONAL EXPERIENCE

Student Parliament, Hamburg University of Technology Hamburg, Germany
Finance committee member *May 1996 – April 1998*

- Approved and revised budget proposals. Informed students about the European credit transfer system.

German Army Heide, Germany
Compulsory military service in the Army Medical Corps *October 1994 – September 1995*

PROFESSIONAL MEMBERSHIPS

American Chemical Society. Member 2006 – present

Computational Molecular Science and Engineering Forum. Member 2005 – present

American Institute of Chemical Engineers. Member 2003 – present

Alumni Society of the Charitable Trust of the German Industry. Member 2001 – present

REFERENCES

Professor Donald G. Truhlar
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Hamburg University of Technology
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Professor Alexis T. Bell
Department of Chemical Engineering
UC Berkeley
201 Gilman Hall
Berkeley, CA 94720
USA
Phone: (510) 642-1536
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Professor Nigel Seaton
Department of Chemical Engineering
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Additional references available upon request.

PUBLICATIONS

[13] 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. *Journal of Chemical Theory Computation in press*

[12] Heyden, A., Truhlar, D. G., A conservative algorithm for an adaptive change of resolution in mixed atomistic / coarse-grained multiscale simulations. *Journal of Chemical Theory Computation* **2008**, 4, 217-221.

[11] 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. *Journal of Catalysis* **2007**, 248, 213-225.

[10] Heyden, A., Lin, H., Truhlar, D. G., Adaptive partitioning in combined quantum mechanical and molecular mechanical calculations of potential energy functions for multiscale simulations. *Journal of Physical Chemistry B* **2007**, 111, 2231-2241.

[9] 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. *Journal of Physical Chemistry C* **2007**, 111, 2092-2101.

[8] 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. *Journal of Physical Chemistry B* **2006**, 110, 17096-17114.

[7] Shao, Y., Kussman, J., Gilbert, A. T., O'Neill, D. P., Wang, T., Herbert, J. M., Chien, S. H., Rassolov, V., Adamson, R., Byrd, E. F. C., Dreuw, A., Furlani, T. R., Hirata, S., Khalliulin, R. Z., Lee, M. S., Peters, B., Rhee, Y. M., Sherrill, C. D., Woodcock, H. L., Chakraborty, A. K., Warshel, A., Krylov, A. I., Molnar, L. F., Ochsenfeld, C., Slipchenko, L. V., Distasio Jr., R. A., Beran, G. J. O., Lin, C. Y., Sodt, A., Maslen, P., Austin, B., Daschle, H., Dunietz, B. D., Gwaltney, S. R., Hsu, C. P., Klunzinger, P., Liang, W., Proynov, E. I., Ritchie, J., Simmonett, A. C., Zhang, W., Chipman, D. M., Schaefer III, H. F., Gill, P. M. W., Jung, Y., Brown, S. T., Levchenko, S., Lochan, R. C., Besley, N. A., Van Voorhis, T., Steele, R., Korambath, P., Baker, J., Doerksen, R. J., Dutoi, A. D., Heyden, A., Keil, F. J., Kedziora, G., Lee, A., Nair, N., Pieniazek, P., Rosta, E., Subotnik, J. E., Bell, A. T., Hehre, W., Kong, J., Head-Gordon, M., Advances in methods and algorithms in a modern quantum chemistry program package. *Physical Chemistry Chemical Physics* **2006**, 8, 3172-319.

[6] 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. *Journal of Chemical Physics* **2005**, 123, 224101-14.

[5] 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. *Journal of Catalysis* **2005**, 233, 26-35.

[4] Heyden, A., Peters, B., Bell, A. T., Keil, F. J., Comprehensive DFT Study of Nitrous Oxide Decomposition over Fe-ZSM-5. *Journal of Physical Chemistry B* **2005**, 109, 1857-1873.

[3] 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. *Journal of Chemical Physics* **2004**, 120, 7877-7886.

[2] Heyden, A., Düren, T., Keil, F. J., Study of molecular shape and non-ideality effects on mixture adsorption isotherms of small molecules in carbon nanotubes: A grand canonical Monte Carlo simulation study. *Chemical Engineering Science* **2002**, 57, 2439-2448.

[1] Heyden, A., Düren, T., Kolkowski, M., Keil, F. J., Design of a Pressure Swing Adsorption Module based on Carbon Nanotubes as Adsorbent – A Molecular Modeling Approach. *Hungarian Journal of Industrial Chemistry* **2001**, 29, 95-104.

CONFERENCE PRESENTATIONS AND INVITED SEMINARS

Invited seminar, MPI for Polymer Research, Mainz, Germany December 2007
(Theory Group, Prof. K. Kremer)
[19] A. Heyden: *A conservative algorithm for an adaptive change of resolution in mixed atomistic / coarse-grained multiscale simulations*

AIChE Annual Meeting, Salt Lake City, USA November 2007
[18] A. Heyden, D. G. Truhlar: *A conservative algorithm for an adaptive change of resolution in mixed atomistic / coarse-grained multiscale simulations*

ACS Spring Annual Meeting, Chicago, USA March 2007
[17] A. Heyden, D. G. Truhlar: *Adaptive partitioning in multilevel/multiscale simulations*

AIChE Annual Meeting, San Francisco, USA November 2006
[16] A. Heyden, D. G. Truhlar: *Combining multilevel methods with modern sampling schemes*
[15] A. Heyden, N. Hansen, A. T. Bell, F. J. Keil: *Nitrous oxide decomposition over Fe-ZSM-5 in the presence of nitric oxide: A comprehensive DFT study*

FOMMS 2006, Blaine, WA, USA, Poster presentation July 2006
[14] A. Heyden, N. Hansen, A. T. Bell, F. J. Keil, D. G. Truhlar: *Nitric oxide assisted nitrous oxide decomposition over Fe-ZSM-5 and the dynamically partitioned multilayer method for multilevel simulations*

AIChE Annual Meeting, Cincinnati, USA November 2005
[13] A. Heyden, A. T. Bell, F. J. Keil: *Kinetic modeling of nitrous oxide decomposition on Fe-ZSM-5 Based on Parameters obtained from a comprehensive DFT study*
[12] A. Heyden, A. T. Bell, F. J. Keil: *Efficient methods for finding transition states in chemical reactions: Comparison of improved dimer method and partitioned rational function optimization method*

Invited seminar, Hamburg University of Technology, Hamburg, Germany August 2005
(Mathematics, Prof. H. Voss)
[11] A. Heyden, A. T. Bell, F. J. Keil: *On finding transition states in chemical reactions*

17th IMACS World Congress Scientific Computation, July 2005
Applied Mathematics and Simulation, Paris, France
[10] A. Heyden, A. T. Bell, F. J. Keil: *On finding transition states in chemical reactions*

Invited seminar, Humboldt University, Berlin, Germany February 2005
(Theoretical Chemistry, Prof. J. Sauer)
[9] A. Heyden, A. T. Bell, F. J. Keil: *Comprehensive DFT study of N_2O decomposition and simulation of related experiments over Fe-ZSM-5 from first principles*

Invited seminar, Fritz Haber Institute of the Max Planck Society August 2004
Berlin, Germany (Theory Department, Prof. M. Scheffler)
[8] A. Heyden, B. Peters, A. T. Bell, F.J. Keil: *A comprehensive DFT study of nitrous oxide decomposition over Fe-ZSM-5*

Invited seminar, Ruhr University, Bochum, Germany May 2004
(Theoretical Chemistry, Prof. V. Staemmler)
[7] A. Heyden, A. T. Bell, F. J. Keil: *Microkinetic modeling of catalytic reactions: N_2O dissociation in Fe-ZSM-5*

AIChE Annual Meeting, San Francisco, USA November 2003
[6] A. Heyden, F. J. Keil: *Analyzing the performance of the dimer method for finding transition states on the high-dimensional potential energy surface of the nitrous oxide dissociation on a Fe-ZSM-5 cluster*
[5] A. Heyden, T. Düren, F. J. Keil: *Maxima in multi-component adsorption isotherms in porous media under supercritical and other conditions*

Workshop on Chemical Engineering Mathematics, Bad Honnef, Germany July 2003
[4] A. Heyden, F.J. Keil: *Analyzing the performance of the dimer method for finding transition states on a high-dimensional potential energy surface (PES)*

Invited seminar, Fritz Haber Institute of the Max Planck Society, July 2003
Berlin, Germany (Theory department, Prof. M. Scheffler)
[3] A. Heyden, F. J. Keil: *Analyzing the performance of the dimer method for finding transition states on the high-dimensional potential energy surface of the nitrous oxide dissociation on a Fe-ZSM-5 cluster*

Thermo 2003, Cambridge, UK, Poster presentation April 2003
[2] A. Heyden, T. Düren, F.J. Keil: *Study of molecular shape and non-ideality effects on mixture adsorption isotherms of small molecules in carbon nanotubes*

Workshop on Chemical Engineering Mathematics, Bad Honnef, Germany August 2001
[1] A. Heyden, T. Düren, F.J. Keil: *Design of a pressure swing adsorption module based on carbon nanotubes as adsorbent. – A molecular modeling approach*