

## WILLIAM FREDERICH SCHNEIDER

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### **Education**

1991, Ph.D., The Ohio State University, Chemistry. Dissertation: "Applications of Local Density Functional Methods to Inorganic Chemistry"  
1986, B.Sc. (High Distinction), The University of Michigan-Dearborn, Chemistry, Math Minor

### **Professional Experience**

2009– Professor, Department of Chemical and Biomolecular Engineering, University of Notre Dame  
2009– Concurrent Professor, Department of Chemistry and Biochemistry, University of Notre Dame  
2004–2009 Assoc. Prof., Department of Chemical and Biomolecular Engineering, University of Notre Dame  
2004–2009 Concurrent Assoc. Prof., Department of Chemistry and Biochemistry, University of Notre Dame  
2001–2004 Staff Technical Specialist and group leader, Chemical and Materials Simulation, Ford Motor Co.  
1996–2001 Senior Technical Specialist, Chemistry Department, Ford Motor Company  
1992–1999 Adjunct Lecturer in General, Physical, and Computational Chemistry, University of Michigan–Dearborn  
1995 Adjunct Lecturer in Physical Chemistry, Wayne State University  
1991–1996 Technical Specialist, Chemistry Department, Ford Motor Company

### **Research Interests**

- First-principles simulation of molecular structure, bonding, and reactivity.
- Adsorption and reaction at metal and metal oxide surfaces.
- Surface chemistry and heterogeneous catalysis of energy and environmental processes.
- Particle size, support, and environmental effects on heterogeneous catalytic activity at the nanoscale.
- Catalysis related to "lean" NO<sub>x</sub> remediation.

### **Selected Professional and Academic Honors**

2009 BP Foundation Outstanding Teacher Award, College of Engineering, University of Notre Dame  
2008 Professional Growth and Scholarship Award, Alumni Society, University of Michigan-Dearborn  
2001 50 Publications Award, Ford Motor Co.  
2001 Arch T. Colwell Outstanding Publication Award, Society of Automotive Engineers  
2000 Technical Achievement Award, Ford Motor Co.  
1999 Invitee, NAE Foundations of Engineering Meeting, Orange County, California  
1997 25 Publications Award, Ford Motor Co.  
1996 Henry Ford Technology Award, Ford Motor Co.  
1995 Technical Achievement Award, Ford Motor Co.  
1986–1989 National Science Foundation Predoctoral Fellow

### **Professional Affiliations**

American Chemical Society (Divisions of Physical and Colloidal and Surface Chemistry)  
American Institute of Chemical Engineers, Chicago Catalysis Club, American Association for the Advancement of Science, Materials Research Society, Sigma Xi

### **Refereed Publications** (92 total, h-index 26)

1. B. E. Bursten and W. F. Schneider, "The Electronic Structure of Asymmetric Metal-Metal Bonds: The d<sup>2</sup>-d<sup>6</sup> Complexes X<sub>4</sub>Mo-Mo(PH<sub>3</sub>)<sub>4</sub> (X = OH, Cl)," *Inorg. Chem.* **1989**, *28*, 3292–3296.
2. R. A. Potts, D. L. Gaj, W. F. Schneider, N. S. Dean, J. W. Kampf, and J. P. Oliver, "Alcoholysis of Nitriles in Gold(III) Complexes: The Structure of EtC(OEt)NH<sub>2</sub><sup>+</sup>[AuCl<sub>4</sub>]<sup>-</sup>," *Polyhedron* **1991**, *10*, 1631–1637.
3. W. F. Schneider, C. K. Narula, H. Nöth, and B. E. Bursten, "Structure and Bonding Trends in Two- and Three-Coordinate Boron Cations," *Inorg. Chem.* **1991**, *30*, 3919–3927.
4. G. S. Tyndall, T. J. Wallington, M. D. Hurley, and W. F. Schneider, "Rate Coefficient for the Reaction of CH<sub>2</sub>OH Radicals with Cl<sub>2</sub> and Infrared Spectra of Chloromethanol and Dichloromethanol," *J. Phys. Chem.* **1993**, *97*, 1576-1582.
5. T. J. Wallington, M. D. Hurley, W. F. Schneider, J. Sehested, and O. J. Nielsen, "Atmospheric Chemistry of CF<sub>3</sub>O Radicals: Reaction with H<sub>2</sub>O," *J. Phys. Chem.* **1993**, *97*, 7606-7611.
6. T. J. Wallington, M. D. Hurley, and W. F. Schneider, "Kinetic Study of the Reaction CF<sub>3</sub>O + O<sub>3</sub> → CF<sub>3</sub>O<sub>2</sub> + O<sub>2</sub>," *Chem. Phys. Lett.*, **1993**, *213*, 442-448.
7. W. F. Schneider and T. J. Wallington, "Ab initio Investigation of the Heats of Formation of Several Trifluoromethyl Compounds," *J. Phys. Chem.*, **1993**, *97*, 12783-12788.
8. T. J. Wallington, M. D. Hurley, W. F. Schneider, J. Sehested, and O. J. Nielsen, "Mechanistic Study of the Gas Phase Reaction of CH<sub>2</sub>FO<sub>2</sub> Radicals with HO<sub>2</sub>," *Chem. Phys. Lett.*, **1994**, *218*, 34-42.
9. W. F. Schneider, "Implementation Strategies for the Ford Waste Minimization Program," *Society of Automotive Engineers Technical Paper*, **1994**, 940543.
10. T. J. Wallington and W. F. Schneider, "The Stratospheric Fate of CF<sub>3</sub>OH," *Environ. Sci. Technol.*, **1994**, *28*, 1198-2000.
11. W. F. Schneider, T. J. Wallington, M. D. Hurley, J. Sehested, and O. J. Nielsen, "Reply to Comment on the Thermochemistry of CF<sub>3</sub>O Radical and CF<sub>3</sub>OH," *J. Phys. Chem.*, **1994**, *98*, 2217-2218.
12. T. J. Wallington, W. F. Schneider, D. R. Worsnop, O. J. Nielsen, J. Sehested, W. Debruyne, and J. A. Shorter, "Atmospheric Chemistry and Environmental Impact of CFC Replacements: HFCs and HCFCs," *Environ. Sci. Technol.*, **1994**, *28*, 320A-326A.
13. W. F. Schneider and T. J. Wallington, "The Thermochemistry of COF<sub>2</sub> and Related Compounds," *J. Phys. Chem.*, **1994**, *98*, 7448-7451.
14. W. F. Schneider, B. I. Nance, and T. J. Wallington, "Bond Strength Trends in Halogenated Methanols: Evidence for Negative Hyperconjugation?," *J. Am. Chem. Soc.*, **1995**, *117*, 478-485.
15. T. E. Møgelberg, O. J. Nielsen, J. Sehested, T. J. Wallington, M. D. Hurley, and W. F. Schneider, "Atmospheric Chemistry of HFC-134a: Kinetic and Mechanistic Study of the CF<sub>3</sub>CFHO<sub>2</sub> + NO<sub>2</sub> Reaction," *Chem. Phys. Lett.*, **1994**, *225*, 375-380.
16. W. F. Schneider, T. J. Wallington, K. Minschwaner, and E. A. Stahlberg, "Atmospheric Chemistry of CF<sub>3</sub>OH: Is Photolysis Important?," *Environ. Sci. Technol.*, **1995**, *28*, 247-250.
17. T. J. Wallington, W. F. Schneider, T. E. Møgelberg, O. J. Nielsen, and J. Sehested, "Atmospheric Chemistry of FCO<sub>x</sub> Radicals: Kinetic and Mechanistic Study of FC(O)<sub>2</sub> + NO<sub>2</sub> Reaction," *Inter. J. Chem. Kinet.*, **1995**, *27*, 391-402.

18. T. J. Wallington, W. F. Schneider, O. J. Nielsen, and J. Sehested, "Comment on the Atmospheric Chemistry of FNO," *J. Phys. Chem.*, **1994**, *98*, 10373.
19. W. F. Schneider and T. J. Wallington, "Comment on Ab Initio Study of the Abstraction Reactions of CF<sub>3</sub>O," *J. Phys. Chem.*, **1995**, *99*, 4353.
20. T. J. Wallington, W. F. Schneider, J. J. Szente, M. M. Maricq, O. J. Nielsen, and J. Sehested, "Atmospheric Chemistry of FNO and FNO<sub>2</sub>: Reactions of FNO with O<sub>3</sub>, O(<sup>3</sup>P), HO<sub>2</sub>, and HCl and the Reaction of FNO<sub>2</sub> with O<sub>3</sub>," *J. Phys. Chem.*, **1995**, *99*, 984-989.
21. T. J. Wallington, W. F. Schneider, J. Sehested, and O. J. Nielsen, "Hydrofluorocarbons and Stratospheric Ozone," *J. Chem. Soc., Faraday Discussions*, **1995**, *100*, 55-64.
22. W. F. Schneider, M. M. Maricq, and J. S. Francisco, "The Vibrational Spectrum of FC(O)O Radical: A Challenging Case for Single-Reference Electron Correlation Methods," *J. Chem. Phys.*, **1995**, *103*, 6601-6607.
23. T. J. Wallington, M. D. Hurley, and W. F. Schneider, "Atmospheric Chemistry of CH<sub>3</sub>Cl: Mechanistic Study of the Reaction of CH<sub>2</sub>ClO<sub>2</sub> Radicals with HO<sub>2</sub>," *Chem. Phys. Lett.*, **1996**, *251*, 164-173.
24. W. F. Schneider, K. C. Hass, R. Ramprasad, and J. B. Adams, "Cluster Models of Cu Binding and CO and NO Adsorption in Cu-Exchanged Zeolites," *J. Phys. Chem.*, **1996**, *100*, 6032-6046.
25. W. F. Schneider, T. J. Wallington, and R. E. Huie, "Energetics and Mechanism of Decomposition of CF<sub>3</sub>OH," *J. Phys. Chem.*, **1996**, *100*, 6097-6103.
26. K. C. Hass and W. F. Schneider, "Reliability of Small Cluster Models for Cu-Exchanged Zeolites," *J. Phys. Chem.*, **1996**, *100*, 9292-9301.
27. G. Rossi and W. F. Schneider, "Accounting for Electron-Electron and Electron-Lattice Effects in Conjugated Chains and Rings," *J. Chem. Phys.*, **1996**, *104*, 9511-9527.
28. V. Catoire, R. Lesclaux, T. J. Wallington, and W. F. Schneider, "Kinetics and Mechanism of the Self-Reactions of CCl<sub>3</sub>O<sub>2</sub> and CHCl<sub>2</sub>O<sub>2</sub> and of their Reactions with HO<sub>2</sub>," *J. Phys. Chem.*, **1996**, *100*, 14356-14371.
29. T. J. Wallington, J. C. Ball, A. M. Straccia, M. D. Hurley, E. W. Kaiser, M. Dill, W. F. Schneider, and M. Bilde, "Kinetics and Mechanism of the Reaction of Cl Atoms with CH<sub>2</sub>CO (Ketene)," *Inter. J. Chem. Kinet.*, **1996**, *28*, 627-635.
30. K. C. Hass and W. F. Schneider, "Density Functional Theory Studies of Cu-Zeolite de-NO<sub>x</sub> Catalysts," *J. Comput. Aided Mat. Design*, **1996**, *3*, 210-212.
31. R. Ramprasad, W. F. Schneider, K. C. Hass, and J. B. Adams, "A Theoretical Study of CO and NO Vibrational Frequencies in Cu-Water Clusters and Implications for Cu-exchanged Zeolites," *J. Phys. Chem. B*, **1997**, *101*, 1940-1949.
32. K. C. Hass, W. F. Schneider, C. M. Estévez, and R. D. Bach, "Density Functional Theory Description of Excited-State Intramolecular Proton Transfer," *Chem. Phys. Lett.*, **1996**, *263*, 414-422.
33. R. Ramprasad, K. C. Hass, W. F. Schneider, and J. B. Adams, "Cu-dinitrosyl Species in Zeolites: A Density Functional Molecular Cluster Study," *J. Phys. Chem. B*, **1997**, *101*, 6903-6913.
34. P. de Sainte Claire, K. C. Hass, W. F. Schneider, and W. L. Hase, "Simulations of Hydrocarbon Adsorption and Penetration on an Aluminum Oxide Surface," *J. Chem. Phys.*, **1997**, *106*, 7331-7342.

35. C. M. Estévez, R. D. Bach, K. C. Hass, and W. F. Schneider, "Novel Structural Modifications Associated with the Highly Efficient Internal Conversion of 2-(2'-hydroxyphenyl)benzotriazole Ultraviolet Stabilizers," *J. Am. Chem. Soc.* **1997**, *119*, 5445–5446.
36. W. F. Schneider, K. C. Hass, R. Ramprasad, and J. B. Adams, "First-Principles Analysis of Elementary Steps in the Catalytic Decomposition of NO by Cu-Exchanged Zeolites," *J. Phys. Chem. B* **1997**, *101*, 4353–4357.
37. T. J. Wallington, W. F. Schneider, J. Sehested, M. Bilde, J. Platz, O. J. Nielsen, and M. J. Molina, "Atmospheric Chemistry of HFE-7100 (C<sub>4</sub>F<sub>9</sub>OCH<sub>3</sub>): Kinetics of Its Reaction with OH Radicals, UV Spectra and Kinetic Data for C<sub>4</sub>F<sub>9</sub>OCH<sub>2</sub>• and C<sub>4</sub>F<sub>9</sub>OCH<sub>2</sub>O<sub>2</sub>• Radicals, and the Atmospheric Fate of C<sub>4</sub>F<sub>9</sub>OCH<sub>2</sub>O• Radicals," *J. Phys. Chem. A* **1997**, *101*, 8264–8274.
38. J. Sehested, L. K. Christensen, O. J. Nielsen, M. Bilde, T. J. Wallington, W. F. Schneider, J. J. Orlando, and G. S. Tyndall, "Atmospheric Chemistry of Acetone: Kinetic Study of the CH<sub>3</sub>C(O)CH<sub>2</sub>O<sub>2</sub> + NO/NO<sub>2</sub> Reactions and Decomposition of CH<sub>3</sub>C(O)CH<sub>2</sub>O<sub>2</sub>NO<sub>2</sub>," *Int. J. Chem. Kinet.* **1998**, *30*, 475–487.
39. W. F. Schneider, K. C. Hass, R. Ramprasad, and J. B. Adams, "Density Functional Theory Study of Transformations of Nitrogen Oxides Catalyzed by Cu-Exchanged Zeolites," *J. Phys. Chem. B* **1998**, *102*, 3692–3705.
40. J. Platz, O. J. Nielsen, J. Sehested, T. J. Wallington, J. C. Ball, M. D. Hurley, A. M. Straccia, W. F. Schneider, and J. Sehested, "Atmospheric Chemistry of the Phenoxy Radical, C<sub>6</sub>H<sub>5</sub>O(•): UV Spectrum and Kinetics of Its Reaction with NO, NO<sub>2</sub>, and O<sub>2</sub>," *J. Phys. Chem. A*, **1998**, *101*, 7964–7974.
41. W. F. Schneider, T. J. Wallington, J. R. Barker, and E. A. Stahlberg, "CF<sub>3</sub>CFHO• Radical: Decomposition vs. Reaction with O<sub>2</sub>," *Ber. Bunsenges. Phys. Chem.* **1998**, *102*, 1850–1856.
42. B. R. Goodman, W. F. Schneider, K. C. Hass, and J. B. Adams, "Theoretical Analysis of Oxygen Bridged Cu Pairs in Cu-Exchanged Zeolites," *Catal. Lett.* **1998**, *56*, 183–188.
43. K. C. Hass, W. F. Schneider, A. Curioni, and W. Andreoni, "Surface Chemistry of Water on Alumina: Reaction Dynamics from First Principles," *Science* **1998**, *282*, 265–268.
44. M. L. Greenfield, G. Mozurkewich, W. F. Schneider, G. D. Bramos, and D. C. Zietlow, "Thermodynamic and Cycle Models for a Low-Pressure CO<sub>2</sub> Refrigeration Cycle," *Society of Automotive Engineers Technical Paper*, **1999**, 010869.
45. K. C. Hass and W. F. Schneider, "Density Functional Studies of Adsorbates in Cu-Exchanged Zeolites: Model Comparisons and SO<sub>x</sub> Binding," *Phys. Chem. Chem. Phys.* **1999**, *1*, 639–648.
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48. B. R. Goodman, K. C. Hass, W. F. Schneider, and J. B. Adams, "Cluster Model Studies of Oxygen-Bridged Cu Pairs in Cu-ZSM-5 Catalysts," *J. Phys. Chem. B* **1999**, *103*, 10452–10460.
49. T. J. Wallington, W. F. Schneider, W. Nelsen, I. Barnes, K. H. Becker, J. Sehested, O. J. Nielsen, "Stability and IR Spectra of Mono-, Di-, and Trichloromethanol," *Chem. Phys. Lett.*, **2000**, *322*, 97–102.
50. G. Mozurkewich, R. D. Roberts, M. L. Greenfield, W. F. Schneider, J. J. Meyer, D. C. Zietlow, and L. I. Stiel, "Cycle-model Assessment of Working Fluids for a Low-Pressure CO<sub>2</sub> Climate Control System," *Society of Automotive Engineers Technical Paper*, **2000**, 010578.

51. K. C. Hass, W. F. Schneider, A. Curioni, and W. Andreoni, "First-Principles Molecular Dynamics Simulations of H<sub>2</sub>O on  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>(0001)," *J. Phys. Chem. B* **2000**, *104*, 5527-5540.
52. B. R. Goodman, K. C. Hass, W. F. Schneider, and J. B. Adams, "Statistical Analysis of Al Distributions and Metal Ion Pairing Probabilities in Zeolites," *Catal. Lett.*, **2000**, *68*, 85-93.
53. D. Sengupta, J. B. Adams, W. F. Schneider, and K. C. Hass, "Theoretical Analysis of N<sub>2</sub>O to N<sub>2</sub> Conversion During the Catalytic Decomposition of NO by Cu-Zeolites," *Catal. Lett.*, **2001**, *74*, 193-199.
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55. X. Lin, N. J. Ramer, A. M. Rappe, K. C. Hass, W. F. Schneider, and B. L. Trout, "Effect of Particle Size on the Adsorption of O and S Atoms on Pt: a Density Functional Theory Study," *J. Phys. Chem. B*, **2001**, *105*, 7739-7747.
56. G. Mozurkewich, M. L. Greenfield, W. F. Schneider, D. C. Zietlow, and J. J. Meyer, "Simulated Performance and Cofluid Dependence of a CO<sub>2</sub>-Cofluid Refrigeration Cycle with Wet Compression," *Int. J. Refrig.*, **2002**, *25*, 1123-1136.
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66. W. F. Schneider, "Qualitative Differences in the Adsorption Chemistry of Acidic (CO<sub>2</sub>, SO<sub>x</sub>) and Amphiphilic (NO<sub>x</sub>) Species on the Alkaline Earth Oxides," *J. Phys. Chem. B*, **2004**, *108*, 273-282.

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81. A. D. Smeltz, R. B. Getman, W. F. Schneider, and F. H. Ribeiro, "Coupled Theoretical and Experimental Analysis of Surface Coverage Effects in Pt-Catalyzed NO and O<sub>2</sub> Reaction to NO<sub>2</sub> on Pt(111)," *Catal. Today*, **2008**, *136*, 84-92.
82. R. B. Getman, Y. Xu., and W. F. Schneider, "Thermodynamics of Environment-Dependent Oxygen Chemisorption on Pt(111)," *J. Phys. Chem. C*, invited Centennial Feature Article, **2008**, *112*, 9559-9572.

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84. L. Xiao and W. F. Schneider, "Surface Environmental Effects on Metal Atom Adsorption on  $\alpha$ -Alumina," *Surf. Sci.*, **2008**, *602*, 3445-3453.
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87. A. A. Phatak, W. N. Delgass, F. H. Ribeiro, and W. F. Schneider, "DFT Comparison of Water Dissociation Steps on Cu, Au, Ni, Pd and Pt," *J. Phys. Chem. C*, **2009**, *113*, 7269–7276.
88. P. Deshlahra, E. E. Wolf, and W. F. Schneider, "A Periodic DFT Study of CO Chemisorption on Pt(111) in the Presence of Uniform Electric Fields," *J. Phys. Chem. A*, **2009**, *113*, 4125–4133.
89. H. Wang, D. Schmidt, and W. F. Schneider, "Intermediates and Spectators in O<sub>2</sub> Dissociation at the RuO<sub>2</sub>(110) Surface," *J. Phys. Chem. C*, **2009**, *113*, 15266-15273.
90. R. B. Getman and W. F. Schneider, "'Coverage-Dependent Microkinetic Model of Pt-Catalyzed NO Oxidation,'" *J. Catal.*, **2009**, submitted for publication.
91. H. Wang and W. F. Schneider, "Molecular Origins of Surface Poisoning during CO Oxidation over RuO<sub>2</sub>(110)," *Surf. Sci.*, **2009**, *603*, L91-L94.
92. L. Xiao and W. F. Schneider, "Influence of  $\alpha$ -Alumina Supports on Oxygen Binding to Pd, Ag, Pt, and Au," *Chem. Phys. Lett.*, **2009**, submitted for publication.

### **Book Chapters and Proceedings**

1. B. E. Bursten and W. F. Schneider, "Theoretical Studies of Multiple Metal-Metal Bonded Compounds," in *Metal-Metal Bonds and Clusters in Chemistry and Catalysis*, J. P. Fackler, ed., Pergamon Press, New York, 1990.
2. W. F. Schneider, R. J. Strittmatter, B. E. Bursten, and D. E. Ellis, "Relativistic DV-X $\alpha$  Studies of Three-Coordinate Actinide Complexes," in *Density Functional Methods in Chemistry*, J. K. Labanowski and J. W. Andzelm, eds., Springer-Verlag, New York, 1990.
3. T. J. Wallington, W. F. Schneider, O. J. Nielsen, J. Sehested, D. R. Worsnop, W. J. DeBruyn, and J. A. Shorter, "Atmospheric Chemistry and Environmental Impact of Hydrofluorocarbons and Hydrochlorofluorocarbons," in *Halon Replacements: Technology and Science*, A. W. Miziolek and W. Tsang, eds., American Chemical Society, Washington, D.C., 1995.
4. K. C. Hass and W. F. Schneider, "Molecular Modeling of Paint Photostabilizers," in *Proceedings of the 7<sup>th</sup> Annual Advanced Coatings Technology Conference*, Engineering Society of Detroit and Society of Automotive Engineers, Detroit, Michigan, September 28-29, 1998.
5. W. F. Schneider, K. C. Hass, M. L. Greenfield, C. Wolverton, A. Bogicevic, D. J. Mann, and E. B. Stechel, "Chemical and Materials Simulation at Ford Motor Company," in *Foundations of Molecular Modeling and Simulation*, P. T. Cummings, P. R. Westmoreland, and B. Carnahan, eds., AIChE Symposium Series No. 325, Volume 97, 2001, pp. 19 - 25.

6. W. F. Schneider, "Fundamental Concepts in NO<sub>x</sub> Catalysis Simulation," in *Environmental Catalysis*, V. Grassian, ed., CRC Press: Boca Raton, 2005.
7. Y. Xu, W. A. Shelton, Jr., and W. F. Schneider, "Theoretical Aspects of Oxide Particle Stability and Chemical Reactivity," in *Synthesis and Application of Oxide Nanoparticles and Nanostructures*, M. Fernandez-Garcia and J. A. Rodriguez, eds., Wiley & Sons, New York, 2007.
8. V. H. Grassian, et al., "Chemistry for a Sustainable Future," Viewpoint article, *Environ. Sci. Technol.* July 15, 2007, 4840-4846.
9. E. Mindrup and W. F. Schneider, "Computational Comparison of Tethering Strategies for Amine Functionalized Ionic Liquids," in ACS Symposium Series, K. Seddon, R. Rogers, and N. Plechkova, eds., American Chemical Society, Washington, D.C., 2009, in press.

### **Invited Presentations**

1. "Metal-Ligand Interactions in Three-Coordinate Actinide(III) Complexes," XIVth International Conference on Organometallic Chemistry, Wayne State University, Detroit, Michigan, August 19–24, 1990.
2. "Atmospheric Chemistry of CFC Replacements: Physical Chemistry in the Real World," Wayne State University, December 8, 1993.
3. "Molecular Models of Copper Zeolites for Lean-NO<sub>x</sub> Catalysis," University of Illinois, February 13, 1995.
4. "Nitrosyl and Carbonyl Complexes of Copper as Models of NO and CO Adsorption in Copper Zeolites," American Chemical Society Central Regional Meeting, Akron, Ohio, May 31–June 2, 1995.
5. "DFT Studies of Cluster Models for Cu-ZSM-5 Lean-NO<sub>x</sub> Catalyst," MSI Materials Science Symposium, Philadelphia, Pennsylvania, September 24–27, 1995.
6. "Current Problems and Applications in Density-Functional Electronic Structure Theory," Institute for Mathematics and Its Applications, University of Minnesota, Minneapolis, Minnesota, November 17, 1995.
7. "Molecular Modeling of Cu-ZSM-5 Lean NO<sub>x</sub> Catalysts," Hope College, Holland, Michigan, December 1, 1995.
8. "Molecular Modeling of Cu-ZSM-5 Lean NO<sub>x</sub> Catalysts," Calvin College, Grand Rapids, Michigan, November 30, 1995.
9. "Molecular Modeling of Cu-ZSM-5 Lean NO<sub>x</sub> Catalysts," Michigan State University, East Lansing, Michigan, February 8, 1996.
10. "Applications of Molecular Modeling in the Automotive Industry," Lubrizol Corp., Wickliffe, Ohio, February 13, 1997.
11. "Theoretical Investigation of NO Decomposition and Selective Catalytic Reduction by Cu-Exchanged Zeolites," Physics Seminar, University of Michigan-Dearborn, February 21, 1997.
12. "Theoretical Investigation of NO Decomposition on Cu-Zeolite Catalysts," 37th Sanibel Symposium on Atomic, Molecular, and Condensed Matter Theory, St. Augustine, Florida, March 1-7, 1997.
13. "Theoretical Results on the Mechanism of Catalytic NO Decomposition over Cu Zeolites," American Chemical Society National Meeting, San Francisco, California, April 1997.
14. "A First Principles Molecular Dynamics Study of Water Adsorption on  $\alpha$ -Alumina," American Chemical Society Central Regional Meeting, Cleveland, Ohio, May 29–31, 1997.

15. "Model Studies of Cu-Zeolite Based Lean NO<sub>x</sub> Catalyst," The Ohio State University, November 19, 1998.
16. "A First Principles Molecular Dynamics Study of Water Adsorption on  $\alpha$ -Alumina," The Ohio State University, November 20, 1998.
17. "Density Functional Theory Investigation of NO<sub>x</sub> Reduction with Cu Zeolite Catalysts," American Chemical Society National Meeting, Anaheim, California, March 21–25, 1999.
18. "Insights Into NO<sub>x</sub> Reduction Catalysis From Molecular Modeling," American Chemical Society National Meeting, Anaheim, California, March 21–25, 1999.
19. "First-principles Modeling of Reactions on Oxide Surfaces for Automotive Exhaust Aftertreatment," Materials Research Society National Meeting, San Francisco, California, April 24–27, 2000.
20. "Density Functional Theory Calculations of NO Reduction Pathways in Cu-ZSM-5," Applications of Quantum Mechanics in the Catalysis, Chemicals, and Electronics Industries, MSI Symposium Series, Chicago, Illinois, May 22, 2000.
21. "First-principles Modeling of Reactions on Oxide Surfaces for Automotive Exhaust Aftertreatment," American Chemical Society Northwest/Rocky Mountain Regional Meeting, Idaho Falls, Idaho, June 15–17, 2000.
22. "Molecular Modeling of Automotive Exhaust Catalysts," Green Chemistry and Engineering Conference, National Academy of Sciences, Washington, D.C., June 27–29, 2000.
23. "Molecular Modeling of Automotive Exhaust Catalysts," National Institute of Standards and Technology, June 29, 2000.
24. "Chemical and Materials Simulation at Ford Motor Company," Foundations of Molecular Modeling and Simulation: Applications for Industry, Keystone Resort, Colorado, July 23–28, 2000.
25. "Molecular Modeling of Automotive Exhaust Catalysts," University of Michigan, Department of Chemical Engineering, September 23, 2000.
26. "Plane-wave Pseudopotential Density Functional Theory for Inorganic Systems," American Chemical Society National Meeting, Washington, D.C., August 20–24, 2000.
27. "Chemical and Materials Simulation at Ford Motor Company," Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, Canada, December 8, 2000.
28. "First-Principles Modeling of Reactions on Oxide Surfaces for Automotive Exhaust Aftertreatment," American Chemical Society Great Lakes/Central Regional Meeting, June 13, 2001.
29. "What Can Thermodynamics Teach Us About Lean NO<sub>x</sub> Aftertreatment?" American Chemical Society National Meeting, Orlando, Florida, April 7–11, 2002.
30. "Insights Into Lean NO<sub>x</sub> Aftertreatment: Atomistics to Thermodynamics," Center for Catalysis and Surface Science, Northwestern University, Chicago, Illinois, April 26, 2002.
31. "Current Perspectives on Automotive Emissions," Department of Chemical Engineering, Purdue University, W. Lafayette, Indiana, May 31, 2002.
32. "New Perspectives on Selective NO<sub>x</sub> Adsorption and Catalytic Reduction," Fysikum, University of Stockholm, Stockholm, Sweden, May 30, 2003.

33. "New Perspectives on Selective NO<sub>x</sub> Adsorption and Catalytic Reduction," CAMP, Danish Technical University, Lyngby, Denmark, June 2, 2003.
34. "New Perspectives on Selective NO<sub>x</sub> Adsorption and Catalytic Reduction," Depts. Of Applied Physics and Competence Center for Catalysis, Chalmers University, Göteborg, Sweden, June 3, 2003.
35. "New Perspectives on Selective NO<sub>x</sub> Adsorption and Catalytic Reduction," Pacific Northwest National Laboratory, September 11, 2003.
36. "Cooperative Effects in Chemisorption on Oxides," American Chemical Society National Meeting, Anaheim, California, March 28—April 1, 2004.
37. "New Perspectives on Selective NO<sub>x</sub> Adsorption and Catalytic Reduction," Texas A&M Department of Chemistry, April 8, 2004.
38. "New Perspectives on Selective NO<sub>x</sub> Adsorption and Catalytic Reduction," Virginia Polytechnic University Department of Chemical Engineering, April 27, 2004.
39. "New Perspectives on Selective NO<sub>x</sub> Adsorption and Catalytic Reduction," University of Notre Dame Department of Chemical and Biomolecular Engineering, May 7, 2004.
40. "Environmental Catalysis from First Principles," ExxonMobil Central R&D, Annandale, New Jersey, November 17, 2004.
41. "Environmental Catalysis from First Principles," Oak Ridge National Laboratory, Oak Ridge, Tennessee, November 22, 2004.
42. "Environmental Catalysis from First Principles," University of Notre Dame, Department of Chemistry and Biochemistry, February 10, 2005.
43. "Catalytic Reactivity at the Intersection of Metals and Oxides," Gordon Research Conference on Chemical Reactions at Surfaces, Ventura Beach Marriot, Ventura, California, February 13-18, 2005.
44. "NO<sub>x</sub> removal from lean exhaust: Insights from thermodynamics and kinetics of NO<sub>x</sub> decomposition and thermal reduction with NH<sub>3</sub>," American Chemical Society National Meeting, San Diego, California, March 13-17, 2005.
45. "The Unusual Adsorption and Reaction Chemistry of NO<sub>x</sub> on Oxide Surfaces," American Physical Society National Meeting, Los Angeles, California, March 20-24, 2005.
46. "Environmental Catalysis at the Interface of Metals and Metal Oxides," Department of Energy, Catalysis and Chemical Transformations Contractors' Meeting, Rockville, Maryland, May 18-21, 2005.
47. "The Unusual Adsorption and Reaction Chemistry of NO<sub>x</sub>," Morley Award Symposium in Honor of Prof. Bruce Bursten, Cleveland Section of the American Chemical Society, Cleveland, Ohio, May 25, 2005.
48. "Lean NO<sub>x</sub> Aftertreatment from Macroscopic and Atomistic Perspectives," Department of Chemical Engineering, Purdue University, July 26, 2005.
49. "Environmental Catalysis from First Principles," Northwest Indiana Grid Computing meeting, Notre Dame, Indiana, August 16-17, 2005.
50. "Simulating Supported Nanoparticles in Realistic Chemical Environments," Brookhaven National Laboratory Nanocatalysis Workshop, Tarrytown, New York, October 20-22, 2005.

51. "Environmental Catalysis from First Principles," Michigan Catalysis Society symposium, Livonia, Michigan, February 23, 2006.
52. "Environmental Catalysis from First Principles," Argonne National Laboratory, Chicago, Illinois, March 2, 2006.
53. "Environmental Catalysis for First Principles," American Physical Society National Meeting, Baltimore, Maryland, March 13, 2006.
54. "First Principles Simulation of Catalysis at Metal and Oxide Surfaces," Educational Symposium on Heterogeneous Catalysis, Oak Ridge Chapter of ASM International, Oak Ridge, Tennessee, April 4, 2006.
55. "First Principles Simulation of Catalysis at Metal and Oxide Surfaces," CECAM Psi-k Workshop on Catalysis from First Principles, Lyon, France, September 11-14, 2006.
56. "Size Dependent Composition and Catalytic Reactivity of Platinum Clusters from First Principles," American Vacuum Society National Meeting, San Francisco, California, November 12-17, 2006.
57. "Simulating Heterogeneous Catalysis in Realistic Environments," Gordon Research Conference on Chemistry of Hydrocarbon Resources, Ventura, California, January 7-11, 2007.
58. "Environmental Catalysis for First Principles," Condensed Matter Physics Colloquium, Department of Physics, University of Notre Dame, February 16, 2007.
59. "First-Principles Simulation of Inorganic Reactions at Metal and Metal Oxide Surfaces," Inorganic Chemistry Colloquium, Department of Chemistry, University of Notre Dame, February 23, 2007.
60. "To Oxidize or Not to Oxidize: First Principles Insights into the Composition and Reactivity of Heterogeneous Catalysts in Realistic Environments," University of Florida, Department of Chemical Engineering, March 19, 2007.
61. "Oxygen Activation at Metal and Metal Oxide Surfaces," (w/R. B. Getman and H. Wang), Symposium on Computational Electrochemistry for New Energy, American Chemical Society National Meetings, Boston, Massachusetts, August 19-23, 2007.
62. "Metal-Support Interactions in Realistic Environments," (w/L. Xiao, W. Lin, and Y. Xu), Symposium on Electronic structure modeling of heterogeneous catalysis, American Chemical Society National Meeting, Boston, Massachusetts, August 19-23, 2007.
63. "First Principles Simulation of Oxidation Catalysis in Realistic Environments," Catalysis Colloquium, Northwestern University, February 1, 2008.
64. "Environmental effects in binding of metal clusters to oxide surfaces," Symposium on Environmental Interfaces, American Chemical Society National Meeting, New Orleans, Louisiana, April 6 – 10, 2008.
65. "Incorporating Environmental Effects in Computational Catalytic Models," International Workshop on Grand Challenges for Catalysis, University of California-Santa Barbara, California, August 10-15, 2008.
66. "First-Principles Evaluation Of CO<sub>2</sub> Complexation In Functionalized Ionic Liquids," (w/E. Mindrup), Symposium on Ionic Liquids: From Knowledge to Application, American Chemical Society National Meeting, Philadelphia, Pennsylvania, August 17-21, 2008.
67. "Environmental Catalysis from First Principles," Department of Chemical Engineering, Purdue University, January 27, 2009.

68. "What's a Chemist Doing Teaching Chemical Engineering?", University of Michigan-Dearborn, Natural Sciences Colloquium, Dearborn, Michigan, March 13, 2009.
69. "First-principles modeling of coverage-dependent rates of catalytic oxidations," Division of Fuels Chemistry, American Chemical Society National Meeting, Salt Lake City, Utah, March 22-26, 2009.
70. "Environmental Catalysis from First Principles," Department of Chemical and Biological Engineering, University of Wisconsin, Madison, Wisconsin, March 31, 2009.
71. "Ionic Liquids: A New Chemical Platform for CO<sub>2</sub> Separations," Indiana CCTR Advisory Committee Meeting, Indiana University, Bloomington, June 4, 2009.
72. "Bridging the Environment Gap using First-Principles-Based Catalyst Modeling," Center for Nanoscale Materials, Argonne National Laboratory, Chicago, Illinois, June 24, 2009.
73. "Environmental Catalysis from First Principles," The 5th Sino-US Conference of Chemical Engineering, Beijing, China, October 12-16, 2009.

### **Contributed Presentations**

1. R. A. Potts and W. F. Schneider, "Participation of Gold Trichlorides in the Alcoholysis of Nitriles," American Chemical Society National Meeting, Chicago, Illinois, September 8-13, 1985.
2. W. F. Schneider and R. A. Potts, "The Metal Ion Catalyzed Alcoholysis of Nitriles," Metropolitan Detroit Undergraduate Research Conference, Wayne State University, March 21, 1986.
3. W. F. Schneider and B. E. Bursten, "A Discrete Variational  $X\alpha$  Investigation of Analogous Chromium(III) and Uranium(III) Complexes," American Chemical Society Central Regional Meeting, Cleveland, Ohio, May 31-June 2, 1989.
4. W. F. Schneider, R. J. Strittmatter, B. E. Bursten, and D. E. Ellis, "The Bonding and Electronic Structure of ThX<sub>3</sub> and UX<sub>3</sub> Compounds where X= Alkyl, Amide, Alkoxide, and Cyclopentadienyl," American Chemical Society National Meeting, Boston, Massachusetts, April 22-27, 1990.
5. W. F. Schneider, B. E. Bursten, C. K. Narula, and H. Nöth, "*Ab initio* Studies of Three-Coordinate Boron Cations," American Chemical Society National Meeting, Boston, Massachusetts, April 22-27, 1990.
6. W. F. Schneider, R. J. Strittmatter, B. E. Bursten, and D. E. Ellis, "Electronic Structure Variations in Three-Coordinate Thorium and Uranium Organoactinides," Ohio Supercomputer Center Workshop on Theory and Applications of Density Functional Approaches to Chemistry, Columbus, Ohio, May 7-9, 1990.
7. W. F. Schneider, B. E. Bursten, C. K. Narula, and H. Nöth, "Substituent Effects in Two- and Three-Coordinate Boron Cations," 45th Ohio State University Symposium on Molecular Spectroscopy, Columbus, Ohio, June 11-15, 1990.
8. W. F. Schneider, "Applications of Computational Chemistry at Ford Motor Company," University of Michigan-Dearborn, February 12, 1993.
9. W. F. Schneider and T. J. Wallington, "Ab initio Determination of the Thermochemistry of CF<sub>3</sub>-containing Atmospheric Intermediates," American Chemical Society National Meeting, Chicago, Illinois, August 22-27, 1993.
10. W. F. Schneider, "Implementation Strategies for the Ford Waste Minimization Program," Society of Automotive Engineers International Meeting, Detroit, Michigan, February 28 - March 3, 1994.

11. W. F. Schneider and T. J. Wallington, "Atmospheric Chemistry of  $\text{CF}_3\text{O}$  and  $\text{CF}_3\text{OH}$ ," American Chemical Society Joint Central-Great Lakes Regional Meeting, Ann Arbor, Michigan, June 1-3, 1994.
12. W. F. Schneider, K. C. Hass, and R. Ramamurthy, "Nitrosyl and Carbonyl Complexes of Copper as Models of NO and CO Adsorption in Copper Zeolites," American Chemical Society National Meeting, Anaheim, California, April 2-6, 1995.
13. W. F. Schneider, K. C. Hass, R. Ramamurthy, and J. Adams, "Computational Investigation of CO and NO Binding in Cu Zeolites," Michigan Catalysis Society Spring Symposium, Ann Arbor, Michigan, May 3, 1995.
14. K. C. Hass, W. F. Schneider, R. Ramprasad, and J. B. Adams, "Density Functional Theory Studies of Cluster Models for Cu Zeolites," 6th International Conference on the Applications of Density Functional Theory in Chemistry and Physics, Ecole Nationale Supérieure de Chimie de Paris, Paris, France, August 29–September 1, 1995.
15. K. C. Hass, W. F. Schneider, R. Ramprasad, and J. B. Adams, "Density Functional Theory Studies of Cluster Models for Cu Zeolites," Molecular Quantum Mechanics: Methods and Applications, St. Catherine's College, Cambridge, England, September 3–7, 1995.
16. W. F. Schneider and T. J. Wallington, "Applications of Quantum Chemistry to the Atmospheric Chemistry of HFCs," Molecular Quantum Mechanics: Methods and Applications, St. Catherine's College, Cambridge, England, September 3–7, 1995.
17. P. de Sainte Claire, W. F. Schneider, K. C. Hass, and W. L. Hase, "Simulations of Competitive Water/Hydrocarbon Wetting of an Aluminum Oxide Surface," American Chemical Society National Meeting, New Orleans, Louisiana, March 23-28, 1996.
18. W. F. Schneider, "Applications of Computational Thermochemistry to Halocarbon Atmospheric Chemistry," American Chemical Society National Meeting, Orlando, Florida, August 25–29, 1996.
19. W. F. Schneider, K. C. Hass, R. Ramprasad, and J. B. Adams, "Computational Investigations of the Structures, Spectroscopy, and Catalytic Activity of Cu-ZSM-5 Lean- $\text{NO}_x$  Catalysts," American Chemical Society National Meeting, Orlando, Florida, August 25–29, 1996.
20. W. F. Schneider, K. C. Hass, A. Curioni, W. Andreoni, "Structural and Dynamic Investigation of the Water/ $\alpha$ -Alumina Interface," American Chemical Society National Meeting, Dallas, Texas, March 29 - April 2, 1998.
21. W. F. Schneider and K. C. Hass, "Molecular Modeling of Sulfur Adsorption on Metal Oxides," American Institute of Chemical Engineers National Meeting, Dallas, Texas, November 1–5, 1999.
22. W. F. Schneider, K. C. Hass, M. Miletic, and J. Gland, "First Principles Modeling of Reactions on Oxide Surfaces for Automotive Exhaust Aftertreatment," American Chemical Society National Meeting, San Diego, California, April 1–5, 2001.
23. W. F. Schneider, K. C. Hass, M. Miletic, and J. Gland, "First-principles comparison of  $\text{NO}_x$  and  $\text{SO}_x$  storage mechanisms on alkaline earth oxides," DOE Crosscut Workshop on Lean Emissions Reduction Simulation, Ford Motor Company, Dearborn, Michigan, October 16–18, 2001.
24. W. F. Schneider, M. Miletic, K. C. Hass, and J. L. Gland, "Dramatic cooperative effects in chemisorption of  $\text{NO}_x$  on oxide surfaces," American Vacuum Society National Meeting, San Francisco, California, October 29–November 2, 2001.

25. W. F. Schneider, K. C. Hass, M. Miletic, and J. L. Gland, "Dramatic Cooperative Effects in the Chemisorption of NO<sub>x</sub> on Oxide Surfaces," American Chemical Society National Meeting, Orlando, Florida, April 7–11, 2002.
26. W. F. Schneider, "Molecular Models of Chemisorption on Oxide Surfaces," (Organizer) 7<sup>th</sup> Annual Mesilla Workshop, Mesilla, New Mexico, February 9–12, 2003.
27. W. F. Schneider, "Cooperative Adsorption of NO<sub>x</sub> on Metal Oxides," American Institute of Chemical Engineers National Meeting, Austin, Texas, November 8–12, 2004.
28. W. F. Schneider, "Mechanistics of Oxidation on Oxide Catalysts," American Institute of Chemical Engineers National Meeting, Austin, Texas, November 8–12, 2004.
29. W. F. Schneider, "Oxidations at Metal Oxide Surfaces," North American Catalysis Society Meeting, Philadelphia, Pennsylvania, May 22-27, 2005.
30. W. F. Schneider, "Simulating catalysis in realistic environments," American Chemical Society National Meeting, Atlanta, Georgia, March 26-30, 2006.
31. W. F. Schneider, "Simulating supported catalysts in realistic environments," American Chemical Society National Meeting, Chicago, Illinois, March 25-29, 2007.
32. W. F. Schneider, R. B. Getman, B. S. Mun, R. M. Rioux, W.S. Epling, D. Zemlyanov, A. D. Smeltz, W.N. Delgass, and F.H. Ribeiro, "Coupled Theoretical and Experimental Analysis of Surface Coverage Effects in Pt-catalyzed NO Oxidation," 20<sup>th</sup> North American Catalysis Society Meeting, Houston, Texas, June 17-22, 2007.
33. W. F. Schneider and A. Ranea, "First-principles Simulation of Aqueous NDMA Reduction at Metal Surfaces," American Chemical Society National Meeting, New Orleans, Louisiana, April 10, 2008.
34. W. F. Schneider and A. Ranea, "Simulation Insights into Catalytic NDMA Reduction at Metal Surfaces," American Institute of Chemical Engineers Annual Meeting, Philadelphia, Pennsylvania, November 16-20, 2008.
35. W. F. Schneider, "Convergence between theory and experiment for catalytic NO oxidation," Physical Division, American Chemical Society National Meeting, Salt Lake City, Utah, March 22-26, 2009.
36. W. F. Schneider and V. A. Ranea, "Molecular-level simulation of NDMA decomposition and reduction at metal surfaces," Materials Research Society Spring Meeting, San Francisco, California, April 13-17, 2009.
37. W. F. Schneider, V. A. Ranea, and I. Carmichael, "Molecular simulation of steps in water adsorption and dissociation at the  $\alpha$ -alumina(0001) surface," Materials Research Society Spring Meeting, San Francisco, California, April 13-17, 2009.
38. W. F. Schneider, R. B. Getman, and A. Phatak, "First-principles catalyst design: Incorporating the effects of surface coverage," Materials Research Society Spring Meeting, San Francisco, California, April 13-17, 2009.
39. W. F. Schneider, "First-Principles Modeling of Coverage-Dependent Rates of Catalytic Oxidations," Great Lakes Regional Meeting, American Chemical Society, May 15, 2009.
40. W. F. Schneider, R. B. Getman, A. Phatak, D. J. Schmidt, H. Wang, and Y. Xu, "Bridging the Environment Gap Using First-Principles-Based Catalyst Modeling," 21<sup>st</sup> North American Catalysis Society Meeting, San Francisco, California, June 7-12, 2009.

### **Patents**

M. L. Greenfield, J. J. Meyer, G. Mozurkewich, W. F. Schneider, L. I. Stiel, "Cofluids for use with carbon dioxide refrigerant," United States Patent 6,415,614, granted July 2002.

### **Funding History**

1. Department of Energy, National Energy Technology Laboratory, "University Computational Materials Consortium," \$68,500, January 1, 2006-December 31, 2006.
2. ExxonMobil Research and Engineering Corporation, unrestricted gift, \$15,000, December 2005.
3. Ford Motor Company, unrestricted gift, \$10,000, September 2006.
4. Department of Energy, Basis Energy Science, "Towards Realistic Models of Heterogeneous Catalysis: Simulations of Redox Catalysis from First Principles," \$420,000, September 1, 2006-August 31, 2009.
5. Department of Energy, National Energy Technology Laboratory, "Ionic Liquids: Breakthrough Absorption Technology for Post-Combustion CO<sub>2</sub> Capture," joint with Profs. J. Brennecke and E. Maginn, \$3,519,265 (\$2,461,605 DOE portion), July 2007-June 2010.
6. National Science Foundation, Science and Technology Center investigator, "The *WaterCAMPWSS*: The Center of Advanced Materials for the Purification of Water with Systems," \$120,000, August 2007-July 2009.
7. National Science Foundation, "Collaborative Research: Predictive Modeling of Surface Catalysis with Multiple Adsorbate Species," \$300,000, September 2007-August 2010.
8. Notre Dame Energy Center, "Towards Simulating Chemical and Photochemical Reactions for Clean Energy: Methodologies for the Solid-Aqueous Interface," joint with Profs. S. Corcelli and K. Newman, \$40,000, September 2008-December 2009.
9. National Science Foundation, "Catalytic Nanodiode," joint with Profs. E. E. Wolf and G. Bernstein, \$371,938, January 1, 2009 – December 31, 2011.

### **Current Graduate Students**

Hangyao Wang (2006 Chemical Engineering), Ph.D. dissertation "Simulation of Catalytic Oxidation over Transition Metal Oxides" to be defended in Fall 2009.

Elaine Mindrup, (2007 Chemical Engineering), dissertation "First-principles Discovery of Chemically Complexing Ionic Liquids"

David Schmidt, (2008 Chemical Engineering), dissertation "Cluster Expansions for Quantitative Analysis of Adsorbate-Adsorbate Interactions"

Mandelle Danser (2009 Chemistry)

Dorrell McCalman (2009 Chemical Engineering)

Jason Bray (2009 Chemical Engineering)

### **Current Post-doctoral Associates**

Dr. Chao Wu

### **Past Graduate Students and Post-Docs**

Dr. Rachel Getman. Ph.D. dissertation, "First Principles Models of NO Oxidation Catalysis," May 2009. Currently post-doc at Northwestern University.

Wenguang Lin, M.Sc. thesis "DFT Simulations of Re<sub>3</sub> Metal Cluster Binding on Alumina in Hydrogen Environments," December 2008. Currently Notre Dame Business School.

Dr. Ye Xu, currently staff scientist, Oak Ridge National Laboratory and NCMS

Dr. Li Xiao, currently post-doc at University of Pittsburgh

Dr. Abhijit Phatak, currently Intel Corp.

Dr. Victor Ranea, currently Conicet Argentina.

### **Undegraduates Supervised**

Josh Bruce (CBE 2007), Jessica Nadai (CBE 2007), Shawn Coleman (CBE 2009), Nathaniel Menendez (CBE 2009), Andrea Baker (CBE 2009), Thomas Senftle (CBE 2010), Daniel Beyrer (Rose-Hulman, 2011), Miriam Shakalli Tang (CBE 2011)

### **Courses Taught**

Physical Chemistry (Wayne State University; University of Michigan-Dearborn), Winter 1996, Winter 1998

Chemical Engineering Laboratory (UND CBE 30358), Spring 2005 and 2007.

Chemical Reaction Engineering (UND CBE 40445), Fall 2005, 2006, and 2008

Physical Chemistry for Chemical Engineers (UND CHEM 30324), Spring 2006, 2007, 2008, 2009  
Molecular Methods in Computational Thermodynamics and Kinetics (UND CBE 60547), Fall 2007, 2009.

### **Other University Service**

Director of Undergraduate Studies, Department of Chemical and Biomolecular Engineering, Fall 2005–present.  
Advisor, AIChE student affiliate chapter, UND, Fall 2005–present.  
Engineering College Computing Committee, Spring 2007–present.  
Center for Research Computing Faculty Advisory Board, Fall 2008

### **Other Professional Activities**

1998 President, Ford Motor Company Chapter of Sigma Xi  
2000 Organizer, “Industrial Applications of Theoretical Chemistry” symposium, American Chemical Society Fall National Meeting, San Francisco, CA  
2002–2004 Chair, Midgley Award Committee, Detroit Section American Chemical Society  
2003 Organizer, 7th Annual Mesilla Workshop, “Environmental Chemistry at Interfaces,” Mesilla, NM  
2004 Invited participant, *Workshop on Advanced Resources for Catalysis Science*, held at the Pacific Northwest National Laboratory, in Richland, Washington, September 21-22  
2003–2005 Liaison member, Computational Molecular Science and Engineering Forum, American Institute of Chemical Engineering  
2004–2006 At-large member, Executive Committee of the Division of Physical Chemistry, American Chemical Society  
2005–2006 Organizing committee, 2006 Foundations of Engineering meeting, National Academy of Engineering  
2005 Invited speaker, *Workshop on Opportunities in Nanocatalysis*, sponsored by Brookhaven National Laboratory Center for Functional Nanomaterials, Tarrytown, New York, October 19-21.  
2006 Invited participant, *Workshop on Sustainability*, sponsored by the Chemistry Division of the National Science Foundation, Washington, D.C., May 30-June 1.  
2006 Organizer, *Best Practices in Density Functional Theory* symposium, AIChE National Meeting, San Francisco, California  
2006– Advisory Board, *Journal of Physical Chemistry*  
2007 Organizer, *Capturing Complexity in Physical Sciences Simulation*, American Chemical Society Spring National Meeting, Chicago, Illinois  
2007 Invited participant, *Workshop on Basic Research Needs in Catalysis for Energy Applications*, sponsored by the Department of Energy, Bethesda, Maryland, August 6-8.  
2008 Special Program Chair, Computational Molecular Science and Engineering Forum, American Institute of Chemical Engineering Spring 2008 Meeting, New Orleans, Louisiana  
2009 Co-organizer, *Molecular Simulation in and for the Environment*, American Chemical Society Great Lakes Regional Meeting, Chicago, Illinois  
2009-2012 Director, Division of Chemical Reaction Engineering, American Institute of Chemical Engineers

Referee for the Journal of Physical Chemistry, Physical Review, Journal of Catalysis, Journal of the American Chemical Society, Angewandte Chemie, Langmuir, Surface Science, Applied Catalysis, Catalysis Today, International Journal of Quantum Chemistry, Chemical Physics, Journal of Physics. Reviewer for DOE, NSF, NRC, PRF.