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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_x remediation.

Selected Professional and Academic Honors

2011	Fellow of the American Association for the Advancement of Science (AAAS)
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, Catalysis, 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

Peer-reviewed Publications (115 total, h-index 33)

1. B. E. Bursten and W. F. Schneider, "The Electronic Structure of Asymmetric Metal-Metal Bonds: The d^2-d^6 Complexes X_4Mo-$Mo(PH_3)_4$ (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 $EtC(OEt)NH_2]^+[AuCl_4]^-$," *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_2OH Radicals with Cl_2 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_3O Radicals: Reaction with H_2O," *J. Phys. Chem.* **1993**, *97*, 7606-7611.

6. T. J. Wallington, M. D. Hurley, and W. F. Schneider, "Kinetic Study of the Reaction $CF_3O + O_3 \rightarrow CF_3O_2 + O_2$," *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_2FO_2 Radicals with HO_2," *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_3OH," *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_3O Radical and CF_3OH," *J. Phys. Chem.*, **1994**, *98*, 2217-2218.

12. T. J. Wallington, W. F. Schneider, D. R. Worsnop, O. J. Nielsen, J. Sehested, W. Debruyn, 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_2 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 $CF_3CFHO_2 + NO_2$ 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_3OH: 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_x Radicals: Kinetic and Mechanistic Study of $FC(O)_2 + NO_2$ 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_3O," *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_2: Reactions of FNO with O_3, $O(^3P)$, HO_2, and HCl and the Reaction of FNO_2 with O_3," *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_3Cl: Mechanistic Study of the Reaction of CH_2ClO_2 Radicals with HO_2," *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_3OH," *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. Lescleaux, T. J. Wallington, and W. F. Schneider, "Kinetics and Mechanism of the Self-Reactions of CCl_3O_2 and $CHCl_2O_2$ and of their Reactions with HO_2," *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_2CO (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-NOx 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 ($C_4F_9OCH_3$): Kinetics of Its Reaction with OH Radicals, UV Spectra and Kinetic Data for $C_4F_9OCH_2$• and $C_4F_9OCH_2O_2$• Radicals, and the Atmospheric Fate of $C_4F_9OCH_2O$• 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 $CH_3C(O)CH_2O_2$ + NO/NO_2 Reactions and Decomposition of $CH_3C(O)CH_2O_2NO_2$," *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, $C_6H_5O(\bullet)$: UV Spectrum and Kinetics of Its Reaction with NO, NO_2, and O_2," *J. Phys. Chem. A*, **1998**, *101*, 7964-7974.

41. W. F. Schneider, T. J. Wallington, J. R. Barker, and E. A. Stahlberg, "$CF_3CFHO\bullet$ Radical: Decomposition vs. Reaction with O_2," *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_2 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_x Binding," *Phys. Chem. Chem. Phys.* **1999**, *1*, 639-648.

46. K. Bolton, S. B. M. Bosio, W. L. Hase, W. F. Schneider, and K. C. Hass, "Comparison of Explicit and United Atom Models for Alkane Chains Physisorbed on α-Al_2O_3 (0001)," *J. Phys. Chem. B* **1999**, *103*, 3885-3895.

47. D. Sengupta, W. F. Schneider, K. C. Hass, and J. B. Adams, "CO Oxidation Catalyzed by Cu-Exchanged Zeolites: A Density Functional Theory Study," *Catal. Lett.*, **1999**, *61*, 179-186.

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_2 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_2O on α-Al_2O_3(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_2O to N_2 Conversion During the Catalytic Decomposition of NO by Cu-Zeolites," *Catal. Lett.*, **2001**, *74*, 193–199.

54. W. F. Schneider, J. Li, and K. C. Hass, "Combined Computational and Experimental Investigation of SO_x Adsorption on MgO," *J. Phys. Chem. B*, **2001**, *105*, 6972–6979.

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_2-Cofluid Refrigeration Cycle with Wet Compression," *Int. J. Refrig.*, **2002**, *25*, 1123–1136.

57. C. T. Goralski, Jr. and W. F. Schneider, "Analysis of the Thermodynamic Feasibility of NO_x Decomposition Catalysis to Meet Next Generation Vehicle NO_x Emissions Standards," *Appl. Catal. B*, **2002**, *37*, 263–267.

58. C. Arsene, I. Barnes, K. H. Becker, W. F. Schneider, T. J. Wallington, N. Mihalopoulos, and I. V. Patroescu-Klotz, "Formation of Methane Sulfinic Acid in the Gas Phase OH-Radical Initiated Oxidation of Dimethyl Sulfoxide," *Environ. Sci. Technol*. **2002**, 36, 5155–5163.

59. M. Miletic, J. L. Gland, K. C. Hass, and W. F. Schneider, "First-Principles Characterization of NO_x Adsorption on MgO," *J. Phys. Chem. B*, **2003**, *107*, 157–163.

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61. X. Lin, W. F. Schneider, K. C. Hass, and B. L. Trout, "Chemistry of Sulfur Oxides on Transition Metals (I): Configurations, Energetics, Orbital Analyses and Surface Coverage Effects of SO_2 on Pt(111)," *J. Phys. Chem. B* **2002**, *106*, 12575–12583.

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63. M. D. Hurley, W. F. Schneider, T. J. Wallington, D. J. Mann, J. D. DeSain, and C. A. Taatjes, "Kinetics of Elementary Reactions in the Chain Chlorination of Cyclopropane," *J. Phys. Chem. A* **2003**, *107*, 2003–2010.

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65. M. Miletic, J. L. Gland, K. C. Hass, and W. F. Schneider, "Characterization of Adsorption Trends of NO_2, Nitrite, and Nitrate Adsorption on MgO Terraces," *Surf. Sci.*, **2003**, *546*, 75–86.

66. W. F. Schneider, "Qualitative Differences in the Adsorption Chemistry of Acidic (CO_2, SO_x) and Amphiphilic (NO_x) Species on the Alkaline Earth Oxides," *J. Phys. Chem. B*, **2004**, *108*, 273–282.

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68. X. Lin, W. F. Schneider, and B. L. Trout, "Chemistry of Sulfur Oxides on Transition Metals (III): Oxidation of SO_2 and Self-Diffusion of O, SO_2, and SO_3 on Pt(111)," *J. Phys. Chem. B*, **2004**, *108*, 13329–13340.

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77. J. P. Larentzos, W. F. Schneider, and E. J. Maginn, "A transferable force field for water adsorption in cation exchanged titanosilicates," *Ind. Eng. Chem. Res.* **2007**, *46*, 5754-5765.

78. T. Yamanaka, M. Kawasaki, M.D. Hurley, T.J. Wallington, W. F. Schneider, and J. Bruce, "Kinetics and Mechanism of the Gas Phase Reaction of Chlorine Atoms," *Phys. Chem. Chem. Phys.* **2007**, *9*, 4211 - 4217.

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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_2 Reaction to NO_2 on Pt(111)," *Catal. Today*, **2008**, *136*, 84-92.

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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.

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89. H. Wang, D. Schmidt, and W. F. Schneider, "Intermediates and Spectators in O_2 Dissociation at the RuO_2(110) Surface," *J. Phys. Chem. C*, **2009**, *113*, 15266-15273.

90. H. Wang and W. F. Schneider, "Molecular Origins of Surface Poisoning during CO Oxidation over RuO_2(110)," *Surf. Sci.*, **2009**, *603*, L91-L94.

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96. E. Mindrup and W. F. Schneider, "Computational Comparison of Substituted Amine Reactions with CO_2," *ChemSusChem*, **2010**, *3*, 931-938.

97. R. B. Getman and W. F. Schneider, "DFT-Based Coverage-Dependent Model of Pt-Catalyzed NO Oxidation," *ChemCatChem*, **2010**, *2*, 1450-1460.

98. B. E. Gurkan, B. F. Goodrich, E. M. Mindrup, L. E. Ficke, M. Masel, S. Seo, T. P. Senftle, H. Wu, M. F. Glaser, J. K. Shah, E. J. Maginn, J. F. Brennecke, and W. F. Schneider, "Molecular Design of High Capacity, Low Viscosity, Chemically Tunable Ionic Liquids for CO_2 Capture," *J. Phys. Chem. Lett.*, **2010**, *1*, 3494-3499.

99. W. Chen, D. Schmidt, W. F. Schneider, and C. Wolverton, "First-principles Cluster Expansion Study of Missing-row Reconstructions of fcc (110) Surfaces," *Phys. Rev. B* **2011**, *83*, 075415.

100. H. Wang and W. F. Schneider, "Adsorption and Reactions of NO_x on RuO_2(110)", *Catal. Today* **2011**, *165*, 49-55.

101. V. A. Ranea, T. J. Strathmann, J. R. Shapley, and W. F. Schneider, "DFT Comparison of N-Nitrosodimethylamine (NDMA) Decomposition Pathways Over Ni and Pd," *ChemCatChem* **2011**, *3*, 898-903.

102. J. M. Bray and W. F. Schneider, "Potential Energy Surfaces for Oxygen Adsorption, Diffusion, and Dissociation at the Pt(321) Surface," *Langmuir* **2011**, *27*, 8177–8186.

103. W. Chen, D. Schmidt, W. F. Schneider, and C. Wolverton, "Ordering and oxygen adsorption in Au-Pt/Pt(111) surface alloys," *J. Phys. Chem C.* **2011**, *115*, 17915-17924.

104. P. Deshlahra, W. F. Schneider, G. H. Bernstein, and E. E. Wolf, "Direct control of electron transfer to the surface-CO bond on a Pt/TiO_2 catalytic diode," *J. Am. Chem. Soc.* **2011**, *133*, 16459-16467.

105. C. Wu, D. J. Schmidt, C. Wolverton, and W. F. Schneider, "Accurate coverage-dependence incorporated into first-principles kinetic models: Catalytic NO oxidation on Pt(111)," *J. Catal.* **2012**, *286*, 88-94.

106. J.-S. McEwen, T. Anggara, W. F. Schneider, V. F. Kispersky, J. T. Miller, W. N. Delgass, F. H. Ribeiro, "Integrated operando X-ray absorption and DFT characterization of Cu−SSZ-13 exchange sites during the selective catalytic reduction of NO_x with NH_3," *Catal. Today* **2012**, *184*, 129-144.

107. D. Schmidt, W. Chen, C. Wolverton, and W. F. Schneider, "Cluster Expansions of Coverage-Dependent Adsorption: Atomic Oxygen on Pt(111)," *J. Chem. Theory Comp.* **2012**, *8*, 264-273.

108. B. Chaplin, M. Reinhard, W. F. Schneider, C. Schueth, J. R. Shapley, T. Strathmann, and C. J. Werth, "A Critical Review of Pd-Based Catalytic Treatment of Priority Contaminants in Water," *Environ. Sci. Technol.* **2012**, *46*, 3655-3670.

109. H. Wang and W. F. Schneider, "Comparative chemistries of CO and NO oxidation over RuO_2(110): Insights from first principles thermodynamics and kinetics," *Molec. Sim.* **2012**, *38*, 615-630.

110. W. Chen, P. Dalach, W. F. Schneider, and C. Wolverton, "Interplay between subsurface ordering, surface segregation, and adsorption on Pt-Ti(111) near-surface alloys," *Langmuir* **2012**, *28*, 4683-4693.

111. D. C. McCalman, K. H. Kelley, C. J. Werth, J. R. Shapley, and W. F. Schneider, "Aqueous N_2O Reduction with H_2 over Pd-Based Catalyst: Mechanistic Insights from Experiment and Simulation," *Topics Catal.* **2012**, *55*, 300-312.

112. P. Deshlahra, J. Conway, E. E. Wolf, and W. F. Schneider, "Influence of Dipole-Dipole Interactions on Coverage-Dependent Adsorption: CO and NO on Pt(111)," *Langmuir* **2012**, *28*, 8408-8417.

113. W. F. Schneider, "Configurational control in catalysis: Perspective on Hess et al., One-dimensional confinement in heterogeneous catalysis: Trapped oxygen on RuO_2(110) model catalysts," *Surf. Sci.* **2012**, *606*, 1351–1352.

114. C. Wu, T. P. Senftle, and W. F. Schneider, "First-Principles-Guided Design of Ionic Liquids for CO_2 Capture," *Phys. Chem. Chem. Phys.*, **2012**, *14*, 13163-13170.

115. J.-S. McEwen, J. Bray, C. Wu, and W. F. Schneider, "New insights into the dissociation pathway of a single O_2 molecule on a Pt(111) surface from first principles," *Phys. Chem. Chem. Phys.*, **2012**, in press.

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-Xα 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 7th 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_x 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., 2010.

10. B. E. Gurkan, J. C. de la Fuente, E. M. Mindrup, L. E. Ficke, B. F. Goodrich, E. A. Price, W. F. Schneider, E. J. Maginn, and J. F. Brennecke, "Chemically Complexing Ionic Liquids For Post-Combustion CO_2 Capture," Clearwater Clean Coal Conference, Clearwater, Florida, May 2010.

11. J. M. Bray and W. F. Schneider, "First-Principles Thermodynamic Models In Heterogeneous Catalysis," in *Computational Catalysis*, M. Janik and A. Asthagiri, eds., Royal Society of Chemistry, 2012.

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_x 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_x 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_x Catalysts," Hope College, Holland, Michigan, December 1, 1995.

8. "Molecular Modeling of Cu-ZSM-5 Lean NO_x Catalysts," Calvin College, Grand Rapids, Michigan, November 30, 1995.

9. "Molecular Modeling of Cu-ZSM-5 Lean NO_x 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 α-Alumina," American Chemical Society Central Regional Meeting, Cleveland, Ohio, May 29–31, 1997.

15. "Model Studies of Cu-Zeolite Based Lean NO_x Catalyst," The Ohio State University, November 19, 1998.

16. "A First Principles Molecular Dynamics Study of Water Adsorption on α-Alumina," The Ohio State University, November 20, 1998.

17. "Density Functional Theory Investigation of NO_x Reduction with Cu Zeolite Catalysts," American Chemical Society National Meeting, Anaheim, California, March 21–25, 1999.

18. "Insights Into NO_x 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 Automtive 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_x Aftertreatment?" American Chemical Society National Meeting, Orlando, Florida, April 7–11, 2002.

30. "Insights Into Lean NO_x 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_x Adsorption and Catalytic Reduction," Fysikum, University of Stockholm, Stockholm, Sweden, May 30, 2003.

33. "New Perspectives on Selective NO_x Adsorption and Catalytic Reduction," CAMP, Danish Technical University, Lyngby, Denmark, June 2, 2003.

34. "New Perspectives on Selective NO_x 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_x 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_x Adsorption and Catalytic Reduction," Texas A&M Department of Chemistry, April 8, 2004.

38. "New Perspectives on Selective NO_x Adsorption and Catalytic Reduction," Virginia Polytechnic University Department of Chemical Engineering, April 27, 2004.

39. "New Perspectives on Selective NO_x 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_x removal from lean exhaust: Insights from thermodynamics and kinetics of NO_x decomposition and thermal reduction with NH_3," American Chemical Society National Meeting, San Diego, California, March 13-17, 2005.

45. "The Unusual Adsorption and Reaction Chemistry of NO_x 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_x," Morley Award Symposium in Honor of Prof. Bruce Bursten, Cleveland Section of the American Chemical Society, Cleveland, Ohio, May 25, 2005.

48. "Lean NO_x 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 Workship, 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_2 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_2 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 (withdrawn due to illness).

74. “What’s a Chemist Doing Teaching Chemical Engineering?”, Valparaiso University, Physics Colloquium, Valparaiso, Indiana, September 25, 2009.

75. “Ionic Liquids: A New Chemical Platform for CO_2 Separations,” Pacific Northwest National Laboratory, Richland, Washington, January 7, 2010.

76. “Environmental Catalysis from First Principles,” Department of Chemistry, University of Wisconsin, Madison, Wisconsin, January 19, 2010.

77. "(Exploiting?) Surface Ordering Effects in Catalysis," Catalytic Materials by Design workshop, University of Notre Dame, January 27-30, 2010.

78. "Ionic Liquids: A New Chemical Platform for CO_2 Separations," Indiana University, Bloomington, Indiana, February 25, 2010.

79. "Environmental Catalysis from First Principles," Workshop on Heterogeneous Catalysis, Indiana University, Bloomington, Indiana, February 26, 2010.

80. "Quantifying the Effects of Surface Coverage on the Rates of Catalytic Oxidations," Division of Fuels Chemistry, American Chemical Society National Meeting, San Francisco, California, March 21-25, 2010.

81. "Environmental Catalysis from First Principles," Philadelphia Catalysis Club Annual Meeting, Philadelphia, Pennsylvania, May 13, 2010.

82. "Capturing the Effects of Surface Coverage on Catalytic Reaction Rates," Gordon Conference on Catalysis, Colby-Sawyer College, New London, New Hampshire, June 27–July 2, 2010.

83. "Ionic Liquids for CO_2 Capture from First-Principles," CECAM workshop on Carbon Capture, Lausanne, Switzerland, July 26-28, 2010.

84. "First-principles investigation of nitrogen oxide catalytic reductions for environmental applications," Division of Environmental Chemistry, American Chemical Society National Meeting, Boston, Massachusetts, August 22–26, 2010.

85. "Exploring the effects of coverage on the statistics and rates of surface reactions," Free University of Brussels, Department of Physics, September 10, 2010.

86. "Exploring the effects of coverage on the statistics and rates of surface reactions," Psi-k 2010 conference, Berlin, Germany, September 12-16, 2010.

87. "Exploring the effects of coverage on the statistics and rates of surface reactions," Åarhus University, Department of Physics, September 17, 2010.

88. "Environmental Catalysis from First Principles," General Motors Research Laboratory, Warren, Michigan, August 8, 2011.

89. "Basis site approach to calculating rates and rate derivatives of coverage-sensitive reactions," Division of Fuel Chemistry, American Chemical Society National Meeting, Denver, Colorado, August 28–September 1, 2011.

90. "Selective catalytic reduction of NOx by ammonia on metal-exchanged zeolite catalysts," Division of Fuel Chemistry, American Chemical Society National Meeting, Denver, Colorado, August 28–September 1, 2011.

91. "Environmental Catalysis from First Principles," Department of Chemical Engineering, Penn State University, State College, Pennsylvania, September 22, 2011.

92. Environmental Catalysis at the Boundary Between Metals and Oxides," Division of Chemical Physics, American Physical Society, Boston, Massachusetts, February 27 – March 2, 2012.

93. "Accurate coverage-dependence incorporated into first-principles kinetic models," Division of Catalysis, American Chemical Society, San Diego, California, March 2012.

94. "First-principles thermodynamics of active sites in Cu-SSZ-13 NOx reduction catalysts," Division of Energy and Fuels, American Chemical Society, San Diego, California, March 2012.

95. "NO_x Catalysis from the Bottom Up," Michigan Catalysis Society, Livonia, Michigan, April 19, 2012.

96. "NO_x Catalysis from the Bottom Up," Brookhaven National Laboratory, Brookhaven, New York, April 26, 2012.

97. "First principles simulation of intermediate steps in nitrate reduction on metal catalysts," Division of Environmental Chemistry, American Chemical Society, Philadelphia, Pennsylvania, August 20, 2012.

98. "Configurational Control in Catalysis," Symposium on the Future of Catalysis, Stanford Linear Accelerator Laboratory, September 27, 2012.

99. "Chemically Complexing Ionic Liquids for Pre-Combustion CO_2 Capture," Global Climate and Energy Project Annual Meeting, Stanford, California, October 10, 2012.

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 Xα 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_3 and UX_3 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_3-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 CF_3O and CF_3OH," 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 Competetive 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-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 NO_x and 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 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_x 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) 7th Annual Mesilla Workshop, Mesilla, New Mexico, February 9–12, 2003.

27. W. F. Schneider, "Cooperative Adsorption of NO_x 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," 20th 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 α-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," 21st North American Catalysis Society Meeting, San Francisco, California, June 7-12, 2009.

41. W. F. Schneider and E. Mindrup, "First-principles Design of Functionalized Ionic Liquids for CO_2 Separations," Division of Physical Chemistry, American Chemical Society National Meeting, San Francisco, California, March 21-25, 2010.

42. W. F. Schneider and E. Mindrup, "AHA! Computational design of aprotic heterocyclic anions for ionic-liquid-based CO_2 separations," Division of Fuel Chemistry, American Chemical Society National Meeting, Boston, Massachusetts, August 22-26, 2010.

43. W. F. Schneider, E. Mindrup, and C. Wu, "Computational Design of Aprotic Heterocyclic Anions (AHAs) for Ionic-Liquid-Based CO2 Separations," North American Catalysis Society Meeting, Detroit, Michigan, June 5-10, 2011.

44. W. F. Schneider and C. Wu, "Theoretical investigation of Nitrogen-Heterocyclic Carbenes as reversible CO2 capture reagents," Division of Physical Chemistry, American Chemical Society, San Diego, California, March 2012.

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.

W. F. Schneider, J. F. Brennecke, E. J. Maginn, E. Mindrup, B. Gurkan, E. Price, and B. Goodrich, "Ionic Liquid Comprising Heteroaromatic Anions," provisional patent filed November 3, 2009.

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_2 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," $180,000, August 2007-July 2010.
7. National Science Foundation, "Collaborative Research: Predictive Modeling of Surface Catalysis with Multiple Adsorbate Species," $300,000, September 2007-August 2010.
8. National Science Foundation, "Catalytic Nanodiode," joint with Profs. E. E. Wolf and G. Bernstein, $371,938, January 1, 2009 – December 31, 2011.
9. Department of Energy, Basic Energy Sciences, "Catalyst Design by Discovery Informatics," Notre Dame portion $195,692, September 1, 2009–August 31, 2012.
10. Department of Energy, Basic Energy Science, "Towards Realistic Reaction Environments in Catalysis Simulation," $465,000, November 1, 2009 – October 31, 2012.
11. National Science Foundation, "GOALI: Collaborative Research: Understanding Perovskite-Based NO Oxidation Catalysts via Coupled Experimental and Computational Analysis," $245,000, August 1, 2010-July 31, 2013.
12. Department of Energy, ARPA-e, "Compact, Efficient Air Conditioning with Ionic Liquid Based Refrigerants," lead PI, $2,800,000, October 1, 2010 – September 30, 2013.
13. Department of Energy, ARPA-e, "CO_2 Capture with Ionic Liquids Involving Phase Change," co-PI, $2,559,569, July 1, 2010 – June 30, 2013.
14. Department of Energy, National Energy Technology Laboratory, "Passive NOx Removal Catalysis Research," lead PI, $900,000, September 1, 2010 – August 31, 2013.
15. Stanford Global Climate and Energy Project, "Chemically-Complexing Ionic Liquids for Pre-Combustion CO2 Capture," co-PI, $1,877,871, September 1, 2012 – August 31, 2015.

Current Graduate Students

David Schmidt, (2008 Chemical Enginering), dissertation "Cluster Expansions for Quantitative Analysis of Adsorbate-Adsorbate Interactions"
Dorrell McCalman (2009 Chemical Enginering)
Jason Bray (2009 Chemical Enginering)
John Clay (2010 Chemical Engineering)
Michael Penninger (2011 Chemical Engineering)
Atun Anggara (2011 Chemical Enginering)
Michelle Morton (2012 Chemistry)
Laura Herder (2012 Chemistry)

Current Post-doctoral Associates

Dr. Sonia Antony
Dr. TaeBum Lee
Dr. Katie Maerzke
Dr. Vladimir Pomogaev
Dr. Shuguang Zhang

Past Graduate Students and Post-Docs

Dr. Elaine Mindrup, Ph. D. dissertation "Discovery of New Ionic Liquids for CO_2 Capture," May 2011.
Mandelle Danser, M. Sc. Thesis "Beyond the Gas Phase: Towards Modeling Bulk Ionic Liquids with a Comparison of Density Functional Tight Binding (DFTB) to Density Functional Theory (DFT)," December 2010.
Dr. Hangyao Wang, Ph.D. dissertation "Simulation of Catalytic Oxidation over Transition Metal Oxides," September 2009. Currently research scientist, Dow Chemical Company.
Dr. Rachel Getman. Ph.D. dissertation, "First Principles Models of NO Oxidation Catalysis," May 2009. Currently Assistant Professor, Clemson University.
Wenguang Lin, M.Sc. thesis "DFT Simulations of Re_3 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 Accelrys Corp.
Dr. Abhijit Phatak, currently Intel Corp.
Dr. Victor Ranea, currently Conicet Argentina.
Prof. Bhabani Mallik, Asst. Prof., Indian Institute of Technology Hyderabad, India
Dr. Chao Wu, research professor, Xi'an Jiaotong University

Dr. Zhengzheng Chen, currently post-doctoral fellow, UCLA
Prof. Jean-Sabin McEwen, Asst. Prof., Washington State University

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), Martin Beres (CBE 2010), Kevin McNamara (CBE 2012), Steven Woltornist (Franciscan University, 2011), Nicklas Hjalmarsson (RIT Sweden, 2012), Mark Sullivan (CBE 2012), Jonathon Conway (CBE 2011), Jennifer Smith (CBE 2012), Ryan Anderson (CBE 2013), Allison Hamman (CBE 2012), Anna-Maria Eriksson (RIT Sweden, 2012), Brian Brady (Penn State 2014)

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 Graduate Admissions, Department of Chemical and Biomolecular Engineering, 2010-.
Director of Undergraduate Studies, Department of Chemical and Biomolecular Engineering, Fall 2005–2009.
Advisor, AIChE student affiliate chapter, UND, Fall 2005-2009.
Engineering College Computing Committee, Spring 2007-2009.
Center for Research Computing Faculty Advisory Board, Fall 2008, 2012

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
2009–2011	External Advisory Board, *Sunshine to Petrol* program, Sandia National Laboratory.
2009-2012	Director, Division of Chemical Reaction Engineering, American Institute of Chemical Engineers
2010	Co-organizer, *Carbon Capture Workshop: Beyond 2020*, DOE Basic Energy Sciences, Washington, DC.
2012	Organizer, "Physical Chemistry of CO_2 Separations," Division of Physical Chemistry, American Chemical Society, San Diego, California, March 25-29, 2012.

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, Environmental Science and Technology. Reviewer for DOE, NSF, NRC, PRF.