[1]BIOGRAPHICAL SKETCH

NAME	TITLE
Thanh Nguyen Truong	Professor of Chemistry

EDUCATION

North Dakota State University	B.S.	1985	Chemistry
University of Minnesota	Ph.D.	1990	Physical Chemistry
University of Houston	NSF Postdoctoral Fellow	1990-92	Physical Chemistry

PROFESSIONAL EXPERIENCE

(7/1/92 - 6/30/97) Assistant Professor
(7/1/97 - 6/30/02) Associate Professor
(7/1/02 - Present) Professor
Department of Chemistry, University of Utah

HONORS AND AWARDS

1993-1998	National Science Foundation Young Investigator Award
1993	Outstanding Community Service Award by the Asian Association of Utah
1990-1992	National Science Foundation Postdoctoral Fellowship
1988-1989	University of Minnesota Doctoral Dissertation Fellowship
1987-1988	Dow Chemical Graduate Fellowship
1985	American Institute of Chemists Award
1985	Phi Kappa Phi honor society
1984-1985	Federation of Societies for Coating Technology Scholarship for outstanding performance in chemistry
1982-1984	Ernest T. Trigg Foundation Scholarships for outstanding performance in chemistry
1982-1983	Phi Eta Sigma honor society
1982-1983	Alpha Lambda Delta honor society
1982-1983	SCM Foundation Scholarship for outstanding performing in chemistry
1982-1983	The Eivind Horvik Memorial Award for Scholarship in Physics
1982	Chemical Rubber Company Achievement Award

AFFILIATIONS

American Chemical Society
American Physical Society
American Institute of Chemical Engineering

PROFESSIONAL ACTIVITIES

- Organized the West Coast Theoretical Chemistry Conference, Salt Lake City, June 2000.
- Co-organized the Symposium on Molecular Modeling and Simulation of Reaction Mechanisms, Kinetics, and Catalysis, ACS National meeting in Orlando, Spring 2002.
- Co-organized the Conference on Computational Chemical Dynamics: From Gas-Phase to Condensed-Phased Systems, Oct. 7-9, 2004, University of Minnesota, Minneapolis, Minnesota.
- Reviewer for Journal of Chemical Physics, Journal of Physical Chemistry, Journal of American Chemical Society, Journal of Organic Chemistry, Journal of Computational Chemistry, International Journal of Chemical Kinetics, Physical Chemistry Chemical Physics, Journal of Molecular Simulations, Surface Science, Energy and Fuels, Carbon, Journal of Chemical

Information and Computer Sciences, Journal of Molecular Catalysis, Theoretical Chemistry Accounts.

(10/22/04)

GENERAL RESEARCH INTERESTS

Development and application of theoretical and computational methods for studying structure, reactivity, spectroscopy of chemical processes in gas phase, in solution, at solid-gas and solid-liquid interfaces, in zeolies, and in biological systems. Development and application of grid enabled cyber-infrastructure for research, collaboration, and education in computational science and engineering.

PUBLICATIONS

1. "Theoretical Studies of Polyvinyl-Substituted Carbenium and Silylenium Ions", T. N. Truong, M. S. Gordon, and P. Boudjouk, *Organometallics* **3**, (1984) 484.

2. "Studies of Silicon-Phosphorus Bonding", K. J. Dykema, T. N. Truong, and M. S. Gordon, *Journal of American Chemical Society* **107**, (1985) 4535.

3. "Thermal Decomposition Pathways of Ethane", M. S. Gordon, T. N. Truong, and J. A. Pople, *Chemical Physics Letters* **132**, (1986) 245.

4. "Theoretical Studies of Reactions of H_2SiNH and Its Isomer $HSiNH_2$", T. N. Truong and M. S. Gordon, *Journal of American Chemical Society* **108**, (1986) 1775.

5. "Potential Primary Pyrolysis Processes of Disilane", M. S. Gordon, T. N. Truong, E. K. Bonderson, *Journal of American Chemical Society* **108**, (1986) 1421.

6. "Potential Primary Pyrolysis Processes of Methylsilane", M. S. Gordon, T. N. Truong, *Chemical Physics Letters* **142**, (1987) 110.

7. "Surface Diffusion of Hydrogen on Copper: The Effect of Phonon-Adsorbate Coupling on the Diffusion Rate", T. N. Truong and D. G. Truhlar, *Journal of Physical Chemistry* **91**, (1987) 6229.

8. "Surface Diffusion of H, D, T on a Metal Surface: The Role of Metal Motions in the Kinetic Isotope Effects", T. N. Truong and D. G. Truhlar, *Journal of Chemical Physics* **88**, (1988) 6611.

9. "Embedded Diatomics-in-Molecules (EDIM): A Method to Include Delocalized Electronic Interactions in the Treatment of Covalent Chemical Reactions at Metal Surfaces", T. N. Truong, D. G. Truhlar, and B. C. Garrett, *Journal of Physical Chemistry* **93**, (1989) 8227.

10. "Application of the Large-Curvature Tunneling Approximation to Polyatomic Molecules: Abstraction of H or D by Methyl Radical", B. C. Garrett, T. Joseph, T. N. Truong, and D. G. Truhlar, *Chemical Physics* **136**, (1989) 271.

11. "Transition State Structure, Barrier Height, and Vibrational Frequencies for the Reaction Cl + CH_4 ↔ HCl + CH_3", T. N. Truong, D. G. Truhlar, K. K. Baldridge, M. S. Gordon, and R. Steckler, *Journal of Chemical Physics* **90**, (1989) 7137.

12. "Calculation of Rate Constants and Kinetic Isotope Effects of Dissociative Chemisorption of H_2 and D_2 on Ni (100), (110), and (111) Surfaces', T. N. Truong, G. Hancock, and D. G. Truhlar, *Surface Science* **214**, (1989) 523.

13. "The Effects of Steps and Surface Coverage on the Rates and Kinetic Isotope Effects for Reactions Catalyzed by Metallic Surfaces: Chemisorption of H_2 on Ni Surfaces", T. N. Truong and D. G. Truhlar, *Journal of Physical Chemistry* **94**, (1990) 8262.

(10/22/04)

14. "The Effects of Steps, Coupling to Substrate Vibrations, and Surface Coverage on the Surface Diffusion Rates and Kinetic Isotope Effects: Hydrogen Diffusion on Ni", T. N. Truong and D. G. Truhlar, *Journal of Chemical Physics* **93**, (1990) 2125.

15. "*Ab Initio* Transition State Theory Calculations of the Reaction Rate for OH + CH_4 ↔ H_2O + CH_3", T. N. Truong and D. G. Truhlar, *Journal of Chemical Physics* **93**, (1990) 1761.

16. "A New *Ab Initio* Potential Energy Surface for H on Ru(0001) and Its Use for Variational Transition State Theory and Semiclassical Tunneling Calculations of the Surface Diffusion of H and D", T. N. Truong, D. G. Truhlar, J. R. Chelikowsky, and M. Y. Chou, *Journal of Physical Chemistry* **94**, (1990) 1973.

17. "Variational Transition State Theory with Multidimensional Semiclassical Ground-State Transmission Coefficients: Applications to Secondary Deuterium Kinetic Isotope Effects in Reactions Involving Methane and Chloromethane", D. G. Truhlar, D.-h. Lu, S. C. Tucker, X. G. Zhao, A. Gonzalez-Lafont, T. N. Truong, D. Maurice, Y.-P. Liu, and G. C. Lynch, in the ACS Symposium Series **502**, (1992) pg. 16 on *Isotope Effects in Chemical Reactions and Photodissociation Processes*, edited by J. A. Kaye, based on a symposium held April 18-19, 1991.

18. "Direct Dynamics Study of Intramolecular Proton Transfer in Hydrogenoxalate Anion", T. N. Truong and J. A. McCammon, *Journal of American Chemical Society* **113**, (1991) 7504.

19. "Interpolated Variational Transition State Theory: Practical Methods for Estimating Variational Transition State Properties and Tunneling Contributions in Electronic Structure Calculations of Chemical Reaction Rates", A. Gonzalez-Lafont, T. N. Truong, and D. G. Truhlar, *Journal of Chemical Physics* **95**, (1991) 8875.

20. "POLYRATE: A Computer Program for Calculation of Chemical Reaction Rates for Polyatomics (version 2.5)", D.-h. Lu, T. N. Truong, A. D. Isaacson, S. N. Rai, G. C. Hancock, J. G. Lauderdale, T. Joseph, V. S. Melissas, and D. G. Truhlar, B. C. Garrett, and R. Steckler, *Quantum Chemistry Program Exchange Bulletin* **11**, (1991) 13.

21. "Direct Dynamics Calculations with MORATE and NDDO Molecular Orbital Theory with Specific Reaction Parameters", A. Gonzalez-Lafont, T. N. Truong, D. G. Truhlar, *Journal of Physical Chemistry* **95**, (1991) 4618.

22. "The Definition of Reaction Coordinates for Reaction Path Dynamics", G. Natason, B. C. Garrett, T. N. Truong, T. Joseph, and D. G. Truhlar, *Journal of Chemical Physics* **94**, (1991) 7875.

23. "POLYRATE 4: a New Version of a Computer Program for the Calculation of Chemical Reaction Rates for Polyatomics", D.-h. Lu, T. N. Truong, V. S. Melissas, G. C. Lynch, Y.-P. Liu, B. C. Garrett, R. Steckler, A. D. Isaacson, S. N. Rai, G. C. Hancock, J. G. Lauderdale, T. Joseph, and D. G. Truhlar, *Computer Physics Communications* **71**, (1992) 235.

24. "A Combined Quantum-Classical Dynamics Method for Calculating Thermal Rate Constants of Chemical Reactions in Solution", T. N. Truong, J. A. McCammon, D. Kouri, and D. K. Hoffman, *Journal of Chemical Physics* **96**, (1992) 8136.

25. "Ab Initio Studies and Quantum-Classical Molecular Dynamics Simulations for Proton Transfer Processes in Model Systems and in Enzymes", P. Bala, B. Lesyng, T. N. Truong, J. A.

McCammon, in the NATO ASI Series volume on *The Role of Computational Models and Theories in Biotechnology*, edited by J. Bertran (Kluwer, Dorcrecht, 1992), pg. 299.

26. "Comparative Study of Time Dependent Quantum Mechanical Wavepacket Evolution Methods", T. N. Truong, J. J. Tanner, P. Bala, J. A. McCammon, D. J. Kouri, B. Lesyng, D. K. Hoffman, *Journal of Chemical Physics* **96**, (1992) 2077.

27. "Molecular Modeling of the Kinetic Isotope Effect for the [1,5]-Sigmatropic Rearrangement of cis-1,3-Pentadiene", Y.-P Liu, G. C. Lynch, T. N. Truong, D.-h. Lu, D. G. Truhlar, and B. C. Garrett, *Journal of American Chemical Society* **115** (1993), 2408.

28. "Acetylcholinesterase: Electrostatic Steering Increases the Rate of Ligand Binding", R. C. Tan, T. N. Truong, J. A. McCammon, *Biochemistry* **32** (1993), 401.

29. "POLYRATE: A Computer Program for the Calculation of Chemical Reaction Rates for Polyatomics (Version 5.0)", Y.-P. Liu, G.C. Lynch, W.-P. Hu, V.S. Melissas, R. Steckler, B.C. Garrett, D. Lu, T.N. Truong, A.D. Isaacson, S.N. Rai, G.C. Hancock, J.C. Lauderdale, T. Joseph, and D.G. Truhlar, *Quantum Chemistry Program Exchange Bulletin* **13** (1993), 28.

30. "MORATE: A Program for Direct Dynamics Calculations of Chemical Reaction Rates by Semiempirical Molecular Orbital Theory", T. N. Truong, D.-h. Lu, G. C. Lynch, Y.-P. Liu, V. S. Mellissas, J. J. P. Stewart, R. Steckler, B. C. Garrett, A. D. Isaacson, A. Gonzalez-Lafont, S. N. Rai, G. C. Hancock, T. Joseph, and D. G. Truhlar, *Computer Physics Communications* **75** (1993), 143.

31. "A Test of Density Functional Theory for Dative Bonding Systems", T. A. Holme and T. N. Truong, *Chemical Physics Letters* **215** (1993), 53.

32. "A Direct *Ab Initio* Dynamics Approach for Calculating Thermal Rate Constants Using Variational Transition State Theory and Multidimensional Semiclassical Tunneling Methods. An Application to the $CH_4 + H_2 \leftrightarrow CH_3 + H_2$ Reaction," T. N. Truong, *Journal of Chemical Physics* **100** (1994), 8014.

33. "A New Direct *Ab Initio* Dynamics Method for Calculating Thermal Ratio Constants from Density Functional Theory," T. N. Truong and W. Duncan, *Journal of Chemical Physics*, **101** (1994), 7408.

34. "Direct *Ab Initio* Dynamics Calculations of Thermal Rate Constants and Kinetic Isotope Effects for the $H + H_2O \leftrightarrow OH + H_2$ Reaction", T. N. Truong and T. J. Evans, *Journal of Physical Chemistry* **98** (1994), 9558.

35. "Direct *Ab Initio* Dynamics Studies of Proton Transfer in Hydrogen Bond Systems", R. L. Bell and T.N. Truong, *Journal of Chemical Physics*, **101** (1994), 10442.

36. "Direct *Ab Initio* Dynamics Methods for Calculating Thermal Rates of Polyatomic Reactions", Thanh N. Truong, Wendell T. Duncan and Robert L. Bell, in the ACS Symposium Series volume on *Density Functional Theory in Chemistry*, edited by B. B. Laird, R. Ross and T. Ziegler, based on a symposium held in Anaheim, CA on April 2-6, 1995, ACS, Washington, D.C., 1996.

37. "Thermal and Vibrational-State Selected Rates of the $CH_4 + Cl \leftrightarrow HCl + CH_3$ Reaction", W.T. Duncan and T.N. Truong, *Journal of Chemical Physics*, **103** (1995), 9642.

38. "POLYRATE 6.5: A new version of a computer program for the calculation of chemical reaction rates for polyatomics," Rozeanne Steckler, Wei-Ping Hu, Yi-Ping Liu, Gillian C. Lynch, Bruce C. Garrett, Alan D. Isaacson, Vasilios S. Melissas, Da-hong Lu, Thanh N. Truong, Sachchida N. Rai, Gene C. Hancock, J.G. Lauderdale, Tomi Joseph, Donald G. Truhlar, *Computer Physics Communications*, **88** (1995), 341.

39. "A new method for incorporating solvent effect into the classical, ab initio molecular orbital and density functional theory frameworks for arbitrary shape solute", T.N. Truong and E.V. Stefanovich, *Chem. Phys. Lett.* **240** (1995), 253.

40. "Optimized atomic radii for quantum dielectric continuum solvation models," E.V. Stefanovich and T.N. Truong, *Chemical Physics Letters*, **244** (1995), 65.

41. "Analytical First and Second Energy Derivatives of the Generalized Conductorlike Screening Model for Free Energy of Solvation of Solute", T.N. Truong and E.V. Stefanovich, *Journal of Chemical Physics*, **103** (1995), 3709.

42. "Hydration Effects on Reaction Profiles: An *Ab Initio* Dielectric Continuum Study of the SN_2 Cl^- + CH_3Cl Reaction," T.N. Truong and E.V. Stefanovich, *Journal of Physical Chemistry*, **99** (1995), 14700.

43. "Direct *Ab Initio* Dynamics Studies of Vibrational-State Selected Reaction Rate of the OH + H_2 ↔ H + H_2O Reaction", T.N. Truong, *Journal of Chemical Physics*, **102** (1995), 5335.

44. "Correlation Between the Madelung Field and the Reactivity of the MgO Low-coordinated Surface Sites," E. Stefanovich and T.N. Truong, *Journal of Chemical Physics*, **102** (1995), 5071.

45. "*Ab Initio* and Density Functional Theory Studies of Proton Transfer in Multiple Hydrogen Bond Systems", Q. Zhang, R. Bell, and T. N. Truong, *Journal of Physical Chemistry*, **99** (1995), 592.

46. "Generalized Conductor-like Screening Model (GCOSMO) for Solvation: An Assessment of Its Accuracy and Applicability," T.N. Truong, U.N. Nguyen and E.V. Stefanovich, *International Journal of Quantum Chemistry*, **30** (1996), 403.

47. "An *Ab Initio* Study of Solvent Effects in Vibrational Spectra," E.V. Stefanovich and T.N. Truong, *J. Chem. Phys*., **105** (1996), 2961.

48. "Development of a Perturbative Approach for Monte Carlo Simulations Using a Hybrid *Ab Initio* QM/MM Method," T.N. Truong and E.V. Stefanovich, *Chemical Physics Letters*, **256** (1996), 348.

49. "Embedded Density Functional Approach for Calculations of Adsorption on Ionic Crystals," E. Stefanovich and T.N. Truong, *Journal of Chemical Physics*, **104** (1996), 2946.

50. "Microsolvation of Cl Anion by Water Clusters: Perturbative Monte Carlo Simulations Using a Hybrid HF/MM Potential", T.N. Truong and E.V. Stefanovich, *Chemical Physics*, **218** (1997) 31.

51. "Primary and Solvent Kinetic Isotope Effects in Water-Assisted Tautomerization of Formamidine: An *Ab Initio* Direct Dynamics Study", R.L. Bell and T.N. Truong, *Journal of Physical Chemistry A*, **101** (1997) 7802.

52. "A General Methodology for Quantum Modeling of Free-Energy Profile of Reactions in Solution: An Application to the Menshutkin NH_3 + CH_3Cl Reaction in Water," T. N. Truong, T.-T. T. Truong, and E. V. Stefanovich, *Journal of Chemical Physics*, **107** (1997), 1881.

53. "An *Ab Initio* Study on the Oxidative Coupling of Methane Over Lithium-Doped MgO Catalyst: Surface Defects and Mechanism," M.A. Johnson, E.V. Stefanovich and T.N. Truong, *Journal of Physical Chemistry B*, **101** (1997), 3196.

54. "A Theoretical Approach for Modeling Reactivity at Solid-Liquid Interfaces," E.V. Stefanovich and T.N. Truong, *Journal of Chemical Physics*, **106** (1997), 7700.

55. "A Direct *Ab Initio* Dynamics Study of the Water-Assisted Tautomerization of Formamide," R.L. Bell, D.L. Taveras, T.N. Truong, and J. Simons, *International Journal of Quantum Chemistry*, **63** (1997), 861.

56. "Thermal Rates of Hydrogen Exchange of Methane with Zeolite: A Direct *ab Initio* Dynamics Study on the Importance of Quantum Tunneling Effects," T. N. Truong, *Journal of Physical Chemistry B*, **101** (1997), 2750.

57. "Solvent Effects on Structure and Reaction Mechanism: A Theoretical Study of [2+2] Polar Cycloaddition between Ketene and Imine", T. N. Truong, *Journal of Physical Chemistry B*, **102** (1998) 7877.

58. "Theoretical Studies of Solid-Liquid Interfaces: Molecular Interactions at the MgO(001)-Water Interface", M.E. Johnson, E.V. Stefanovich, and T.N. Truong, *Journal of Physical Chemistry B*, **102** (1998) 6391.

59. "Quantum Modelling of Reactions in Solution: An Overview of the Dielectric Continuum Methodology", T.N. Truong, *International Reviews in Physical Chemistry*, **17** (1998) 525.

60. "Optimizing Efficiency of Perturbative Monte Carlo Method", T.J. Evans and T.N. Truong, *Journal of Computational Chemistry*, **19** (1998) 1632.

61. "Ab Initio Study of the Stabilization of Multiply Charged Anions in Water", E.V. Stefanovich, A.I. Boldyrev, T.N. Truong, and J. Simons, *Journal of Physical Chemistry B*, **102** (1998) 4205.

62. "TheRate: Program for *Ab Initio* Direct Dynamics Calculations of Thermal and Vibrational-State-Selected Rate Constants", W.T. Duncan, R.L. Bell, T.N. Truong, *Journal of Computational Chemistry*, **19** (1998) 1039.

63. "A Simple Method for Incorporating Madelung Field Effects into Ab Initio Embedded Cluster Calculations of Crystals and Macromolecules", E.V. Stefanovich and T.N. Truong, *Journal of Physical Chemistry B*, **102** (1998) 3018.

64. "A Methodology for Quantum Molecular Modeling of Structure and Reactivity at Solid-Liquid Interfaces", E.V. Stefanovich and T.N. Truong, in "Combined QM/MM Methods and Applications", Edited by J. Gao and M. Thompson, ACS Symposium Series, 1998, Vol 712, p. 92.

65. "A Reaction Class Approach for Modeling Gas Phase Reaction Rates", T.N. Truong, W.T. Duncan, M. Tirtowidjojo, *Physical Chemistry Chemical Physics*, **1** (1999) 1061.

66. "Importance of Polarization in Simulations of Condensed Phased Energetic Materials", M.A. Johnson and T.N. Truong, *Journal of Physical Chemistry B*, **103** (1999) 9392.

67. "High Level *Ab Initio* and Density Functional Theory Evaluation of Combustion Reaction Energetics: NO_2 and HONO Elimination from Dimethylnitramine", M.A. Johnson and T.N. Truong, *Journal of Physical Chemistry* A, **103** (1999) 8840.

68. "Quantum Modeling of Adsorption onto Solid-Gas and Solid-Liquid Interfaces", T.N. Truong, V. Shapovalov, M. Johnson, E.V. Stefanovich, Proceedings of the AIChE 4th Topical Conference on Separations Science and Technology, 1999.

69. "Molecular Modeling of Interactions in Zeolites: An Ab Initio Embedded Cluster Study of NH_3 Adsorption in Chabazite", J.M. Vollmer, E.V. Stefanovich, T.N. Truong, *Journal of Physical Chemistry B*, **103** (1999) 9415.

70. "Direct *Ab Initio* Dynamics Studies of the Hydrogen Abstraction Reactions of Hydrogen Atom with Fluoromethanes", D.K. Maity, W.T. Duncan, T.N. Truong, *Journal of Physical Chemistry A*, **103** (1999) 2152.

71. "A Reaction Class Approach with the Integrated Molecular Orbital + Molecular Orbital (IMOMO) Methodology", T.N. Truong and T.-T.T. Truong, *Chemical Physics Letters*, **314** (1999) 529.

72. "An Approach for Inclusion of Crystal Polarization in Embedded Cluster Calculations: Application to CaF_2", V.E. Puchin, E.V. Stefanovich, and T.N. Truong, *Chemical Physics Letters*, **304** (1999) 258.

73. "*Ab Initio* Study of Water Adsorption on TiO_2(110): Molecular Adsorption Versus Dissociative Chemisorption", E.V. Stefanovich and T.N. Truong, *Chemical Physics Letters* **299** (1999) 623.

74. "Dissociation of Water at the MgO(100)-Water Interface: Comparison of Theory with Experiment", M.A. Johnson, E.V. Stefanovich, and T.N. Truong, *Journal of Physical Chemistry B*, **103** (1999) 3391.

75. "Mechanism and Quantum Tunneling Effects on Inner Hydrogen Atom Transfer in Free Base Porphyrin: A Direct *Ab Initio* Dynamics Study", D.K. Maity, R.L. Bell and T.N. Truong, *Journal of American Chemical Society*, **122** (2000) 897.

76. "Liquid Structure and Metal Oxide-Water Interface: Accuracy of a Three-Dimensional RISM Methodology", V. Shapovalov, T.N. Truong, A. Kovalenko and F. Hirata, *Chemical Physics Letter*, **320** (2000) 186.

77. "Adsorption of Carbon Monoxide in H-ZSM-5 and Li-ZSM-5 Zeolites: An Embedded *Ab Initio* Study", J. Limtrakul, P. Khongpracha, S. Jungsuttiwong, and T.N. Truong, *Journal of Molecular Catalysis A*, **153** (2000) 155.

78. "A Combined Reaction Class Approach with Integrated Molecular Orbital + Molecular Orbital (IMOMO) Methodology: A Practical Tool for Kinetic Modeling", T.N. Truong, D.K. Maity and T.-T.T. Truong, *Journal of Chemical Physics*, **112** (2000) 24.

79. "Thermal Rate Constants of the NO_2 Fission Reaction of Gas Phase α-HMX: A Direct *Ab Initio* Dynamics Study", S. Zhang and T.N. Truong, *Journal of Physical Chemistry A*, **104** (2000) 7304.

80. "Spin Contamination in Hartree-Fock and Density Functional Theory Wavefunctions in Modeling of Adsorption on Graphite", A. Montoya, T.N. Truong and A.F. Sarofim, *Journal of Physical Chemistry A,* **104** (2000) 6108.

81. "Reaction Class Transition State Theory: Hydrogen Abstraction Reactions by Hydrogen Atoms as Test Cases", T.N. Truong, *Journal of Chemical Physics*, **113** (2000) 4957.

82. "Mechanisms of Hydrogen Exchange of Methane with H-Y Zeolite: An *Ab Initio* Study", Journal of American Chemical Society, J.M. Vollmer and T.N. Truong, *Journal of Physical Chemistry B,* **104** (2000) 6308.

83. "Direct *Ab Initio* Dynamics Studies of $N + H_2 \leftrightarrow NH+H$ Reaction", S. Zhang and T.N. Truong, *Journal of Chemical Physics*, **113** (2000) 6149.

84. "Direct *Ab Initio* Dynamics Methodology for Modeling Kinetics of Biological Systems", T.N. Truong and D. K. Maity, in *Computational Chemistry: Reviews of Current Trends*, edited by T. Leszczynski, World Scientific, **5** (2000) 211.

85. "Application of Density Functional Theory to the Study of the Reaction of NO with Char-Bound Nitrogen during Combustion", A. Montoya, T.N. Truong and A.F. Sarofim, *Journal of Physical Chemistry A,* **104** (2000) 8409.

86. "*Ab Initio* Study of Water Adsorption on α-Al_2O_3 (0001) Crystal Surface", V. Shapovalov and T.N. Truong, *Journal of Physical Chemistry B,* **104** (2000) 9859.

87. "Thermochemistry of Solvation: A Self-Consistent Three-Dimensional Reference Interaction Site Model Approach", A. Kovalenko and T.N. Truong, *Journal of Chemical Physics*, **113** (2000) 7458.

88. "Status of Theoretical Modeling of Tautomerization in Free-Base Porphyrin", D.K. Maity and T.N. Truong, *Journal of Porphyrins and Phthalocyanines*, **5** (2001) 289.

89. "CO Desorption from Carbonyl Surface Species in the Gasification of Coal", A. Montoya, T.-T. T. Truong, F. Mondragon, T.N. Truong, *Pre-prints of Symposia – American Chemical Society Division of Fuel Chemistry*, **46** (2001) 215.

90. "CO_2 Adsorption on Carbonaceous Surfaces: A Combined Molecular Modeling and Experimental Study" , A. Montoya, F. Mondragon and T.N. Truong, *Pre-prints of Symposia, American Chemical Society, Division of Fuel Chemistry*, **46** (2001) 217.

91. "Electronic Structure and Chemical Reactivity of Metal Oxides-Water Interfaces", T.N. Truong, M.A. Johnson, and E.V. Stefanovich, in *Structure and Reactivity of Solid-Liquid Interfaces*, W. Halley, Ed., ACS Symposium Series, **789** (2001) 124.

92. "Branching Ratio and Pressure Dependent Rate Constants of Multi-Channel Unimolecular Decomposition of Gas-Phase α-HMX: An Ab Initio Dynamics Study", S. Zhang and T.N. Truong, *Journal of Physical Chemistry A*, **105** (2001) 2427.

93. "Adsorption of Nitrogen Monoxide and Carbon Monoxide on Copper Exchange ZSM-5: A Cluster and Embedded Cluster Study", P. Treesukol, J. Limtrakul and T.N. Truong, *Journal of Physical Chemistry B*, **105** (2001) 2421.

94. "CO Desorption from Oxygen Species on Carbonaceous Surface: 1. Effects of the Local Structure of the Active Site and the Surface Coverage", A. Montoya, T.-T. T. Truong, F. Mondragon and T.N. Truong, *Journal of Physical Chemistry A*, **105** (2001) 6757.

95. "Quantum Mechanical Study of Molecular Weight Growth Process by Combination of Aromatic Molecules", A. Violi, T.N. Truong and A.F. Sarofim, *Combustion and Flame*, **126** (2001) 1506.

96. "Adsorption of Unsaturated Hydrocarbons on Zeolites: The Effects of the Zeolite Framework on Adsorption Properties of Ethylene", J. Limtrakul, T. Nanok, S. Jungsuttiwong, P. Khongpracha and T. N. Truong, *Chemical Physics Letters*, **349** (2001) 161.

97. "A Full Quantum Embedded Cluster Methodology: An Application to Proton Siting in Chabazite" , P. Treesukol, J.P. Lewis, J. Limtrakul, and T.N. Truong, *Chemical Physics Letters*, **350** (2001) 128.

98. "A Theoretical Study of Adsorption of Carbon Monoxide on Ag-ZSM-5 Zeolite" , S. Jungsuttiwong, P. Khongpracha, T.N. Truong, and J. Limtrakul, *Studies in Surface Science and Catalysis*, **135** (2001) 2518.

99. "Coverage Effects on Adsorption of Water in Faujasite: An *Ab Initio* Cluster and Embedded Cluster Study" , J. Limtrakul, S. Nokbin, P. Chuichay, P. Khongpracha, S. Jungsuttiwong, T.N. Truong, *Studies in Surface Science and Catalysis*, **135** (2001) 2469.

100. "Modeling the Desorption of NOx species in the Combustion of Coal" , A. Montoya, F. Mondragon, A.F. Sarofim, T.N. Truong, *Pre-prints of Symposia – American Chemical Society, Division of Fuel Chemistry*, **46** (2001) 363.

101. Computational Strategy for Studying Chemical Processes on Carbonaceous Surfaces" , T.N. Truong, A. Montoya, F. Mondragon, *Pre-prints Symposia – American Chemical Society Division of Fuel Chemistry*, **46** (2001) 367.

102. "Adsorption on Carbonaceous Surfaces: Cost-effective Computational Strategies for Quantum Chemistry Studies of Aromatic Systems", A. Montoya, F. Mondragon, and T.N. Truong, *Carbon*, **40** (2002) 1863.

103. "Kinetics of Nitric Oxide Desorption from Carbonaceous Surfaces," A. Montoya, F. Mondragon, T. N. Truong, *Fuel Processing Technology* **77-78** (2002) 453-458.

104. "First-principles Kinetics for CO Desorption During Gasification of Coal" , A. Montoya, F. Mondragon, and T.N. Truong, *Journal of Physical Chemistry A*, **106** (2002) 4236.

106. "Mechanistic Pathways to Explain H/C Ratio of Soot Precursors," A. Violi, A. F. Sarofim, and T. N. Truong. *Combustion and Science Technology*, **174** (2002) 205.

107. "A Fully Integrated Kinetic Monte Carlo/Molecular Dynamics Approach for the Simulation of Soot Precursor Growth", A. Violi, A Kubota, T. N. Truong, W. J. Pitz, C. K. Westbrook, A. F. Sarofim, Proceeding of the Combustion Institute, 29 (2002) 2343-2349.

(10/22/04)

108. "Oxygen Adsorption on Nitrogen-containing Carbon Surfaces," A. MontoyaJ. O. Gil, F. Mondragon, and T. N. Truong. *Pre-Prints of Symposia - American Chemical Society, Division of Fuel Chemistry*, **47** (2002) 424.

109. "Formation of CO Precursors During Char Gasification with O_2, CO_2 and H_2O," A Montoya, F. Mondragon and TN Truong, *Fuel Processing Technology* **77-78** (2002) 125.

110. Nature of the Excited States of the Rutile TiO_2 (1 1 0) Surface with Adsorbed Water," V. Shapovalov, EV Stefanich and TN Truong, *Surface Science* **498** (2002) L103.

111. "CO_2 Adsorption on Carbonaceous Surface: A Combined Experimental and Theoretical Study", A. Montoya, F. Mondragon, and T.N. Truong, *Carbon*, **41** (2003) 29.

112. "Application of Chemical Graph Theory for Automated Mechanism Generation", A. Ratkiewicz and T.N. Truong, *Journal of Chemical Information and Computer Sciences*, **43** (2003) 36.

113. "Kinetics of Hydrogen Abstraction Reaction Class H + H—C(sp^3): First-Principle Predictions Using the Reaction Class Transition State Theory," S. Zhang and T.N. Truong, *Journal of Physical Chemistry A*, **107** (2003) 1138.

114. "Theoretical study of Mechanism, Thermodynamics and Kinetics of the Decomposition of Gas phase HMX (Octahydro-1,3,5,7-Tetranitro-1,3,5,7-Tetrazocine)", S. Zhang, H.N. Nguyen, and T.N. Truong, *Journal of Physical Chemistry B,* **107** (2003) 2981.

115. "Theoretical Analysis of the Electronic Spectra of Water Adsorbed on the Rutile TiO_2 (110) and MgO (100) Surfaces," V. Shapolav, Yan Wang, Thanh N. Truong. *Chemical Physics Letters*, 375 (2003) 321.

116. "A Coupled RISM/MD or MC Simulation Methodology for Solvation Free Energies", H. Freedman and T.N. Truong, Chemical Physics Letters, 381 (2003) 362.

117. "Density Functional Theory Study of the Ethylene Epoxidation over Ti-substituted Silicalite (TS-1): An Application of Cluster and Embedded Cluster Methods" Jumras Limtrakul, Chan Inntam, and Thanh N. Truong, *Journal of Molecular Catalysis A: Chemical*, **207(2)**, (2004), 139.

118. "Density Functional Theory Study of Carbon-H_2O Reactions during Gasification with Steam. J. F. Espinal, F. Mondragon, and T.N.Truong, *American Chemical Society, Division of Fuel Chemistry*, **49** (2004), 822.

119. "Coupled Reference Interaction Site Model/Simulation Approach for Thermochemistry of Solvation: Theory and Prospects." H. Freedman, and T. N. Truong, *Journal of Chemical Physics* **121,** (2004), 2187.

120. "A DFT Study of Interaction of Carbon Monoxide with Carbonaceous Materials", J. F. Espinal, A. Montoya, F. Mondragon, T. N. Truong, *Journal of Physical Chemistry B* (2004), **108(3)**, 1003-1008.

121. "Theoretical Study of Adsorption of Water Dimer on the Perfect MgO(100) Surface: Molecular Adsorption versus Dissociative Chemisorption", Y. Wang and T.N. Truong, *Journal of Physical Chemistry B* (2004), 108, 3289-3294.

122. "Kinetics of Hydrogen Abstraction Reactions From Polycyclic Aromatic Hydrocarbons by H atoms," A. Violi, T. N. Truong, A. F. Sarofim, *J Physical Chemistry A* (2004), **108**, 4846.

123. "Computational Science and Engineering Online: An Integrated Web-based Environment for Multi-scale Modeling of Complex Reaction Systems", T. N. Truong, T. Cook, M. Nayak, C. Boonyasiriwat, L.-T. T. Tran, and S. Zhang, Proceedings of the 2nd International Conference on Foundations of Molecular Modeling and Simulations. *Molecular Physics* (2004), **102**, 353.

124. "An Integrated Web-based Grid-Computing Environment for Research and Education in Computational Science and Engineering", T. N. Truong, Proceeding of the 37th Annual Simulation Symposium, Arlington, April 18-22, 2004, page 143.

125. "Direct *ab initio* Dynamics Studies of the Reactions of HNO with H and OH radicals", H. M. T. Nguyen, S. Zhang, J. Peeters, T.N. Truong, and M. T. Nguyen, *Chemical Physical Letters* (2004), **388,** 94.

126. "Computational Engineering and Science Program at the University of Utah", C. DeTar, A. L. Fogelson, C. R. Johnson, C. A. Sikorski, and T.N. Truong, Proceeding of the International Conference on Computational Science, Krakow, Polan, June 6-9, 2004, M. Bubak et al. (Eds), (Springer-Verlag, 2004), page 1202.

127. "An Application of Coupled Reference Interaction Site Model (RISM)/Molecular Dynamics (MD) Method to the Conformational Analysis of the Alanine Dipeptide", H. Freedman and T. N. Truong. *Journal of Physical Chemistry*, in press.

128. "A Study of the Tautomic Equilibria of 2-hydroxypyridine/2-oxopyridine and of Cytosine in Water Using the Coupled Reference Interaction Site Model (RISM)/Molecular Dynamics (MD) Approach", H. Freedman and T. N. Truong *Journal of Physical Chemistry*, in press.

129. "A Theoretical Study of Adsorption of Carbon Monoxide and Nitrogen Oxide on Ag-ZSM-5 Zeolite", P. Krongpracha, P. Treesukol, J. Limtrakul, and T. N. Truong. *Journal of Physical Chemistry*, Submitted.

PRESENTATIONS (since 7/1/92)

Invited or Contributed Oral Presentations

1. "Direct Dynamics Calculations of Chemical Reaction Rates," seminar given at Biosym, Inc., April 5, 1993.

2. "Dynamical Studies of Water-Assisted Proton Transfer Reactions." Invited speaker at the 3rd Symposium on Molecular Reaction Dynamics in Condensed Matter, Salt Lake City, Utah, April 6-9, 1994.

3. "Direct *Ab Initio* Dynamics Calculations of Chemical Reaction Rates." Contributed speaker at the Fifteenth Annual West Coast Theoretical Chemistry Conference, Livermore, California, April 27-29, 1994.

4. "Direct *Ab Initio* Dynamics Calculations of Chemical Reaction Rates," seminar given at the Department of Chemistry, University of Copenhagen, Denmark, August 18, 1994.

5. "Direct *Ab Initio* Dynamics Calculations of Chemical Reaction Rates," seminar given at the Department of Chemistry, University of Wisconsin, Milwaukee, Nov. 28, 1994.

6. "Development and Applications of a New Quantum Dielectric Continuum Solvation Model," seminar given at Pacific Northwest Laboratory, Richland, WA, Feb. 24, 1995.

7. "Development and Applications of a New Quantum Dielectric Continuum Solvation Theory," invited talk given at the Center for Computational Engineering, Sandia National Laboratories, Livermore, California, March 20, 1995.

8. "Development and Applications of a New Quantum Dielectric Continuum Solvation Theory," invited talk given at the Department of Chemistry, University of California at San Diego, March 28, 1995.

9. "Direct *Ab Initio* Dynamics Calculations of Classical Reaction Rate Using Density Functional Theory", contributed talk at the 209th ACS meeting, Anaheim, California, April 2-6, 1995.

10. "Development and Applications of a New Quantum Dielectric Continuum Solvation Theory," Seminar given at the Department of Chemistry, University of Houston, May 5, 1995.

11. "Development and Applications of a New Quantum Dielectric Continuum Solvation Theory," invited speaker at ACS 12th Rocky Mountain Regional Meeting, Park City, Utah, June 14-17, 1995.

12. "A Direct *Ab Initio* Dynamics Approach for Predicting Kinetics and Dynamics of Gas-phase Reactions," invited presentation at the High Performance Computational Chemistry Workshop, Pleasant, California, August 13-16, 1995.

13. "Roles of Aqueous Solvent in Proton Transfer Reactions," contributed talk at the 210th ACS Meeting, Chicago, Illinois, August 20-24, 1995.

14. "Development and Applications of a New Dielectric Continuum Solvation Theory," contributed talk at the 210th ACS Meeting, Chicago, Illinois, August 20-24, 1995.

15. "Quantum Molecular Modeling of Solvation," invited talk at Department of Biochemistry, University of Utah, January 14, 1996.

16. "Quantum Modeling of Structure, Reactivity and Spectroscopy in Solution," invited talk at the Department of Chemistry, University of Oregon, January 29, 1996.

17. "Modeling of Reaction Rates and Environmental Effects," invited talk at Pacific Northwest Laboratories, Pasco, Washington, January 30, 1996.

18. "Quantum Molecular Modelling of Solvation," invited presentation at the 36th Sanibel Symposium, Florida, February 22-29, 1996.

19. "Direct *Ab Initio* Dynamics Methods for Predicting Gas-Phase Chemical Reaction Rates," contributed talk given at the American Chemical Society National Meeting, New Orleans, LA, March 24-28, 1996.

20. “Quantum Dielectric Continuum Study of Hydration Effects on Transition States of Reactions in Solution,” contributed talk given at the American Chemical Society National Meeting, New Orleans, LA, March 24-28, 1996.

21. “Molecular Modeling of Chemical Reactions,” invited talk given at the Vietnamese-American Science and Professional Engineering Society Conference on “Contributions of Vietnamese-Americans to Science and Technology in the Past 20 Years,” Los Angeles, CA, March 29-31, 1996.

22. “Quantum Predictive Continuum Studies of Solvent Effects on Conformation and Reaction Profile,” invited presentation at the 13th Rocky Mountain Regional ACS Meeting, Denver, Colorado, June 9-12, 1996.

23. “Quantum Molecular Modeling of Condensed-Phase Chemistry,” invited presentation at the 1996 American Conference on Theoretical Chemistry, Park City, Utah, July 21-25, 1996.

24. “Quantum Molecular Modeling of Condensed Phase Chemistry, invited seminar at the Department of Chemistry, Wayne State University, Michigan, May 17, 1997.

25. “Molecular Modeling of Chemical Reactivity of Zeolites,” invited presentation at the 29th Central Regional Meeting, Midland, Michigan, May 28-30, 1997.

26. “Applications of Density Functional Theory in Condensed-phase Chemistry,” invited presentation at the Symposium on Density Functional Theory and Applications, Duke University, Durham, North Carolina, June 3-7, 1997.

27. "Predicting Kinetics of Chemical Reactions from First Principles: A Robust and Practicle *Ab Initio* Direct Dynamics Methodology", invited presentation at the Third Canadian Computational Conference, University of Alberta, Edmonton, July 19-23, 1997.

28. "Predicting Kinetics of Chemical Reactions from First Principles: A Robust and Practicle *Ab Initio* Direct Dynamics Methodology", invited presentation at the Third Conference on Halon Replacement, AWAFB, Dayton, Ohio, July 22-24, 1997.

29. "*Ab Initio* QM/MM Methodology for Modeling Structure and Reactivity at Solid-Liquid Interfaces"; invited presentation at the American Chemical Society National Meeting, Las Vegas, Aug. 11-18, 1997.

30. "A General Methodology for Quantum Modeling of Free Energy Profiles of Reaction in Solution", invited presentation at the American Chemical Society National Meeting, Las Vegas, Aug. 11-18, 1997.

31. "Quantum Modeling of Reaction Rates and Environmental Effects", invited seminar at Dow Chemical, Freeport, Texas, Oct. 4, 1997.

32. "A New Methodology for Modeling NMR Chemical Shifts in Crystals", contributed talk at the American Chemical Society National Meeting, Boston, Aug. 23-27, 1998.

33. "An Overview of Methodologies for Modeling Reactions in Solution", invited talk at Dow Chemical Company, Freeport, Texas, Oct. 15, 1998.

34. "Quantum Modeling of Structure and Reactivity at Solid-Gas and Solid-Liquid Interfaces", invited talk at the Collaborative Computational Project 1 Meeting at Daresbury Laboratory, Manchester, England, Oct. 30-Nov. 1, 1998.

35. Series of invited talks (5) at Kasetsart University, Bangkok, Thailand, Nov. 9-18, 1998.

36. "Current Trends in Computational Chemistry", invited seminar at the Vietnam Science and Natural Science National Laboratory, Dec. 8, 1998.

37. "Computational Methodologies for First-Principle Prediction of Thermal Rate Constants of Elementary Gas Phase Chemical Reactions", invited seminar at 13th Annual Technical Conference of ASERC, Provo, Utah, Feb. 25, 1999.

38. "Molecular Modeling of Reactions in Zeolites", contributed talk at the American Chemical Society National Meeting, Anaheim, March 21-25, 1999.

39. "Elucidating the Mechanism of the Oxidative Coupling of Methane on the Surface of Lithium-Doped MgO", contributed talk at the American Chemical Society National Meeting, Anaheim, March 21-25, 1999.

40. "Methodologies for Predicting Thermal Rate Constants of Gas-Phase Reactions", invited talk at the American Chemical Society National Meeting, Anaheim, March 21-25, 1999.

41. "Quantum Molecular Modeling of Reactions in Water: A Dielectric Continuum Approach", contributed talk at the American Chemical Society National Meeting, Anaheim, March 21-25, 1999.

42. "Quantum Molecular Modeling of Processes at Metal Oxides-Water Interfaces", contributed talk at the American Chemical Society National Meeting, New Orleans, Aug. 22-27, 1999.

43. "Modeling Kinetics of Gas Phase Reactions", contributed talk at the American Chemical Society National Meeting, New Orleans, Aug. 22-27, 1999.

44. "Molecular Modeling of Zeolite Catalysis and Kinetics of Elementary Chemical Reactions", invited seminar, Dow Chemical Company, October 27, 1999.

45. "Quantum Molecular Modeling of Reactions in Zeolites," contributed talk at the American Institute of Chemical Engineers Annual Meeting, Dallas, November 1, 1999."

46. "Density Functional Theory of Calculations of Proton Mobility in ZSM-5," contributed talk at the American Institute of Chemical Engineers Annual Meeting, Dallas, November 4, 1999.

47. Quantum Modeling of Adsorption at Solid-Gas and Solid-Liquid Interfaces", contribued talk at the American Institute of Chemical Engineers Annual Meeting, Dallas, November 3, 1999.

48. Invited lecture (2) series at the Faculty of Science, Kasetsart University, Bangkok, Thailand, Nov. 16-17, 1999.

49. “Reaction Class Transition State Theory”, contributed talk at the American Physical Society Annual Meeting, Minneapolis, March 23, 2000.

50. "Modeling Mechanism and Kinetics of Complex Combustion System", invited talk at the 220th ACS National Meeting, Washington, DC, Aug. 20-24, 2000.

51. "Theoretical and Computational Chemistry in the New Mellenium, invited talk at the University of Utah College of Science Day, Nov. 18, 2000.

52. "Electronic Structure and Liquid Structure at Metal Oxide-Water Interfaces", invited talk at Pacfichem 2000, Honolulu, Hawaii, Dec. 14-19, 2000.

53. Invited lecture series (3) at the Department of Chemistry, University of Antioquia, Columbia, Oct. 2-8, 20000.

54. "Modeling Mechanism of Complex Chemical Reactions", invited talk at the 2000 Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, Nov. 12-17, 2000.

55. "Quantum Modeling of Proton Mobility in Zeolites", contributed talk at the 2000 Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, Nov. 12-17, 2000.

56. Invited lecture series at the Department of Chemistry, Kasetsart University, Bangkok, Thailand, Feb. 24-26, 2001.

57. "Computational Modeling of Interfacial Phenomena", invited lecture, Department of Physics, Mahidol University, Bangkok, Thailand, Feb. 27, 2001.

58. "Computational Chemistry in the New Millennium: Current Perspectives and Future Outlook", invited lecture, Department of Chemical Engineering, Ho-Chi-Minh City University of Technology, Saigon, Vietnam, Mar. 4, 2001.

59. "Computational Chemistry in the New Millennium: Current Perspectives and Future Outlook", invited lecture, Department of Chemistry, Vietnam's National University, College of Natural Sciences, Saigon, Vietnam, Mar. 5, 2001.

60. "Theoretical Studies of CO Desorption from Char", contributed talk in the Fuel Chemistry Division at the National ACS Meeting, San Diego, April 1-5, 2001.

61. “Modeling the desorption of NOx species in the combustion of coal”, contributed talk at the 222nd ACS National Meeting, Chicago, August 26-30, 2001, in the symposium on Computer Modeling in Fuel Chemistry.

62. “Computational strategy for studying chemical processes on carbonaceous surfaces”, contributed talk with T. N. Truong , A. Montoya , F. Mondragon at 222nd ACS National Meeting in the symposium on Computer Modeling in Fuel Chemistry, Chicago, August 26-30, 2001.

63. “Development of a virtual kinetic laboratory: A step toward global science”, contributed talk at the 222nd ACS National Meeting in the special symposium on Emerging Computational Technologies at the 125th Anniversary of the ACS, Chicago, August 26-30, 2001.

64. “Embedded cluster methodologies for modeling heterogeneous catalysis”, invited talk by T. N. Truong , P. Treesukol , J. Lewis at the 222nd ACS National Meeting in the symposium on QM/MM Methods, Chicago, August 26-30, 2001.

65. “Application of graph theory for automated mechanism generation”, invited talk by A. T. Ratkiewicz , T. N. Truong at the 222nd ACS National Meeting, Chicago, August 26-30, 2001.

66. Invited for Lecture series at the Department of chemistry, Kasetsart University, Bangkok, Thailand Nov 26, 2001.

67. “Molecular Modeling of Coal Gasification,” contributed talk at a Departmental seminar, California State University at Fullerton, Dec. 10, 2001

68. “Molecular Modeling of Heterogeneous Catalysis,” invited lecture at National Tsing Hua University, Mar. 14, 2002.

69. “Recent Advance in Gas-phase Reation Kinetics,” invited lecture at Institute of Atomic and Molecular Sciences of Taiwan, Mar. 15, 2002.

70. “Computational Methods for Modeling Nano-materials,” invited lecture at Mahidol University, Thailand, March 25, 2002.

71. “Recent Advance in Gas-phase Reactions Kinetics,” invited lecture at Kassetsart University, Bangkok, Thailand, March 26, 2002.

72. “Structure and Activity of Metal Oxide Interfaces,” invited lecture at Chulalongkorn University, Thailand, March 27, 2002.

73. "Bridging Fundamental Chemistry and Reaction Engineering," Invited Talk at 223rd American Chemical Society Meeting, Orlando, FL, April 7-11, 2002.

74. Invited Lecture Series at Kassetsart University, July, 2002.

75. Invited Lecture Series at Chulalongkorn University, July, 2002.

76. "Computational Chemistry in the New Millenium," Invited Lecture at Chiang Mai University, Thailand, July 29, 2002.

77. "Modeling reactions on carbonaceous surfaces." Contributed Talk at 224th American Chemical Society Meeting, Boston, MA, August, 2002.

78. "Structure and Relativity of Metal Oxide Interfaces," Invited Lecture at University of Antioquia, Medellin, Colombia, November 28, 2002.

79. "Chemistry of Metal Oxides Interfaces," Invited Seminar at Emory University, Atlanta, GA, February 17 2003.

80. “Mechanism of Methane Formation for Hydrogen Storage in Carbon Single Wall Nanotubes”. Contributed talk at the 225th American Chemical Society Meeting, New Orleans, March 24, 2003.

81. “First-Principles simulations of carbon gasification reactions”, Contributed talk at the 225th American Chemical Society Meeting, New Orleans, March 24, 2003.

82. “Integrated Web-based Environment for Computational Science and Engineering”, Contributed talk at the 225th American Chemical Society Meeting, New Orleans, March 24, 2003.

83. “Molecular Dynamics Simulations of Full-length HIV-I Integrase protein”, Invited seminar at the department of chemistry, Chulalongkorn University, May 8, 2003.

84. “New Perspectives in Computational Chemistry”, Invited seminar at the department of chemistry, Khon Khaen University, Thailand, May 14, 2003.

85. “Molecular Modeling of Carbon Single Wall Nano-tubes”, Invited seminar at the department of physics, Mahidol University, Thailand, May 15, 2003.

86. “Bridging Fundamental Chemistry and Reaction Engineering”, Invited lecture, the 2nd International Conference on Foundations of Molecular Modeling and Simulation, Keystone, July 6-11, 2003.

87. "Computational Science and Engineering Online", Invited presentation for the Computational Engineering and Science Graduate Program Annual Luncheon, University of Utah, March 26, 2004.

88. "A Web-based Grid-computing Environment for Computational Science and Engineering", Contributed presentation at the 227th ACS meeting, March 28-April 2, 2004.

89. "Computational Science and Engineering Online: An Intergrated Web-based Simulation Environment for Computational Science and Engineering", Contributed presentation at the Advanced Simulation Technologies Conference 2004, April 18-22, Arlington, Virginia.

90. Invited Lecturer for the 2nd Thailand National Summer School for Computational Chemistry, Chiang Mai University, Chiang Mai, Thailand, May 9-13, 2004.

91. "Molecular Modeling of Heterogeneous Catalysis", Invited presentation at the Petroleum and Petrochemical College, Chulalongkorn University, Bangkok, Thailand, June 1, 2004.

92. "Computational Methods for Solvation", Invited Lecture at the Faculty of Chemical Engineering, Ho-Chi-Minh City Polytechnical University, Ho-Chi=Minh City, Vietnam, June 10, 2004.

93. "Computational Chemistry: Perspectives and Opportunities", Invited presentation at the Vietnam National Education University, Ho-Chi-Minh City, Vietnam, June 14, 2004.

94. “Computational Science and Engineering Online”, Invited presentation for the Chemistry Division, National Science Foundation, Washington D.C., August 2, 2004.

95. “Computational Science and Engineering Online: Progress and Perspective”, Invited presentation at the NSF CHE Cyber-Enabled Chemistry Workshop, Oct. 3-5, 2004, Washington D.C.

96. “Reaction Class Transition State Theory”, Contributed presentation at the Conference on Computational Chemical Dynamics: From Gas-Phase to Condensed-Phase Systems, Oct. 7-9, 2004, University of Minnesota, Minneapolis, Minnesota.

PATENTS

"Locally Operated Desktop Environment of a Remote Computer System", Thanh N. Truong, US Patent, pending.

FUNDING SUPPORT

History:

(1992 – 1998) University of Utah Start-up Grant
(1993 – 1998) National Science Foundation Young Investigator Award
(1995 – 1998) National Science Foundation Grant
(1998 – 1999) University of Utah Seed Grant
(1998 – 2003) Department of Energy Center for Simulations of Accidental Fires and Explosions. (C-SAFE).
(1998 – 2004) Unrestricted gift from Dow Chemical Company.
(1999 – 2002) National Science Foundation Grant
(2000 – 2001) National Science Foundation – NATO Postdoctoral Fellowship
(2001 – 2002) University of Utah Seed Grant
(2001 – 2003) ACS – Petroleum Research Grant
(2001 – 2003) National Science Foundation Information Technology Research

Current:

Thailand Royal Golden Jubille Ph.D. Award, providing travel expenses for the awarded US professor to Thailand once or twice a year

NSF, "ITR: Development of a Web-based Grid-Computing Environment for Research and Education in Computational Science and Engineering," $3,200,000 total, 8/1/03-7/31/07.

NSF, "Collaborative Research: Polycyclic Aromatic Hydrocarbon Growth Mechanisms in Combustion Involving Cyclopentadiene and Indene," (co-PI) $240,001 total, 5/01/03-4/30-06.

In preparation:

NSF, "Electronic Structure and Reactivity of Oxide Supported Metal Clusters"
ACS-PRF, "Development of a Coupled RISM/Simulation Method for Thermochemistry of Solvation,"
Department of Energy, "First-Principles Chemoinformatics for Combustion of Hydrocarbons"

CURRENT STUDENTS AND ASSOCIATES

Visiting Professor

Dr. Artur Ratkiewicz

Project Manager

Manohar Nayak

Graduate Students:

(10/22/04)

Department of Chemistry

1. Piti Treesukol (Thailand Royal Golden Jubilee Ph.D. Fellowship)
2. Holly Freedman
3. Lam Huynh (Vietnam Education Foundation Fellowship)
4. Pipat Khronpracha (Thailand Royal Golden Jubilee Ph.D. Fellowship)
5. Nawee Kungwan (Thailand Ph.D. Fellowship)
6. Yang Wang
7. Hoa G. Nguyen (Vietnam Education Foundation Fellowship)
8. Ly Le (Vietnam Education Foundation Fellowship)

Computational Science and Engineering Graduate Program

1. Tom Cook
2. Le-Thuy T. Tran
3. Bharath Jannu
4. Priya Mahajan
5. Nhat Nguyen
6. Hung Huynh
7. Chaiwoot boonyasiriwat
8. Shrish Jain

Computer Science Graduate Program

1. Yong Kim

PREVIOUS STUDENTS AND ASSOCIATES

Qi Zhang (Postdoc, 1992-94) (ARUP - biotech)
Robert Bell (Ph.D., 1997) (University of Pittsburgh)
Vladimir Puchin (Postdoc, 1997-1998) (SYNOPSIS)
Eugene V. Stefanovich (Adjunt Assistant Professor, 1994-1998) (SYNOPSIS)
Michael Johnson (Ph.D., 1999) (Lockheed Martin Laboratory)
Dilip Maity (1998-2000) (Bhabha Atomic Research Center)
Wendell Duncan (Ph.D. 1998, Postdoc 1998-2000) (Cogni Tech, SLC)
Andriy Kovalenko (Postdoc, 1999-2000) (Institute of Molecular Science, Japan)
Thanh-Thai T. Truong (B.S., 2000) (Cephelon, SLC)
James Vollmer (Ph.D., 2000) (Argonne National Laboratory)
Shao-wen Zhang (Post Doc., 2000-02) (Beijing University of Technology, China)
Artur Ratkiewicz, (Post Doc., 1999-2002) (University of Bialystok, Poland)
Vladimir Shapovalov (Ph.D., 2002) (University of California Santa Barbara)
Hung Nguyen (BS, 2004) (MIT Biophysics)
Hai Huynh (BS in CS, 2004)
Tim Song (BS in CS, 2004)
Lorelei C. Rao (BS in Graphic Art, 2004)

(10/22/04)