Curriculum Vitae

Haobin Wang
Department of Chemistry
University of Colorado Denver
Campus Box 194, P.O. Box 173364
Denver, CO 80217-3364
Phone: (303) 556-5866 Fax: (303)-556-4776
E-mail: haobin.wang@ucdenver.edu

Professional Preparation:

University of Science & Technology of China	Chemical Physics	B.S. 1991
Wayne State University	Physical Chemistry	Ph.D. 1996
University of California-Berkeley	Theoretical Chemistry	10/96 - 07/01

Appointments:

1996-2001: Postdoctoral Fellow, University of California-Berkeley

2001-2006: Assistant Professor, New Mexico State University

2006-2011: Associate Professor, New Mexico State University

2011-2014: Professor, New Mexico State University

2014-present: Professor and Chair, University of Colorado Denver

Awards:

1987 Outstanding Student Award—First Honor, University of Science and Technology of China.

1989 ELITE Award for Outstanding Experimental Research, University of Science and Technology of China.

1996 Trivich Memorial Award for Research in Physical Chemistry, Department of Chemistry, Wayne State University.

2004 National Science Foundation CAREER award.

2005 University Research Council Award for Creative Scholarly Activity, New Mexico State University.

Professional Society Memberships:

1996-Present: American Chemical Society

List of Publications:

1. H. Wang, L. Zhu and W.L. Hase, "A Model Multidimensional Analytic Potential Energy Function for the $Cl^- \cdots CH_3Br \rightarrow ClCH_3 \cdots Br^-$ Reaction", J. Phys. Chem., **98**, 1608 (1994).
2. H. Wang, G.H. Peslherbe and W.L. Hase, "Trajectory Studies of S_N2 Nucleophilic Substitution. IV. Intramolecular and Unimolecular Dynamics of the $Cl^- \cdots CH_3Br$ and $ClCH_3 \cdots Br^-$ Complexes", J. Am. Chem. Soc., **116**, 9644 (1994).
3. G.H. Peslherbe, H. Wang and W.L. Hase, "Unimolecular Dynamics of $Cl^- \cdots CH_3Cl$ Intermolecular Complexes Formed by $Cl^- + CH_3Cl$ Association", J. Chem. Phys., **102**, 5626 (1995).
4. H. Wang and W.L. Hase, "Statistical Rate Theory Calculations of the Cl^- + $CH_3Br \rightarrow ClCH_3$ + Br^- Rate Constant versus Temperature, Translational Energy, and H(D) Isotopic Substitution", J. Am. Chem. Soc., **117**, 9347 (1995).
5. G.H. Peslherbe, H. Wang and W.L. Hase, "Trajectory Studies of S_N2 Nucleophilic Substitution. V. Semiempirical Direct Dynamics of $Cl^- \cdots CH_3Br$ Unimolecular Decomposition", J. Am. Chem. Soc., **118**, 2257 (1996).
6. H. Wang and W.L. Hase, "Reaction Path Hamiltonian Analysis of the Dynamics for Cl^- + CH_3Br $\rightarrow ClCH_3$ + Br^- S_N2 Nucleophilic Substitution", Chem. Phys. **212**, 247 (1996).
7. B. Nizamov, D.W. Setser, H. Wang, G.H. Peslherbe, and W.L. Hase, "Quasiclassical Trajectory Calculations for the OH and OD + HBr Reactions: Energy Partitioning and Rate Constants", J. Chem. Phys. **105**, 9897 (1996).
8. W.L. Hase, R.J. Duchovic, X. Hu, K.F. Lim, D.-h. Lu, G.H. Peslherbe, K.N. Swamy, S.R. Vande Linde, H. Wang, R.J. Wolf, *VENUS, A General Chemical Dynamics Program*, Quantum Chemistry Program Exchange, **16**, 671 (1996).
9. H. Wang, E.M. Goldfield, and W.L. Hase, "Quantum Dynamical Study of the Cl^- + CH_3Br Reaction", J. Chem. Soc. Faraday Trans. **93**, 737 (1997).
10. J.V. Seeley, R.A. Morris, A.A. Viggiano, H. Wang and W.L. Hase, "Temperature Dependence of the Rate Constants and Branching Ratios for the Reactions of $Cl^-(H_2O)_{0-3}$ with CH_3Br and Thermal Dissociation Rates for $Cl^-(CH_3Br)$", J. Am. Chem. Soc. **119**, 577 (1997).
11. H. Wang and W.L. Hase, "Kinetics of the F^- + CH_3Cl S_N2 Nucleophilic Substitution", J. Am. Chem. Soc. **119**, 3093 (1997).
12. H. Wang and W.L. Hase, "Lyapunov Exponent for the Intramolecular Motion of the $Cl^- \cdot\cdot CH_3Br$ Complex", Int. J. Mass Spectrometry and Ion Process, **167**, 573 (1997).
13. W.L. Hase, P.de-Sainte Claire, G.H. Peslherbe, and H. Wang, "Linear Free Energy of Activation Relationship for Association Reactions", J. Am. Chem. Soc. **119**, 5007 (1997).
14. H. Wang, W.H. Thompson, and W.H. Miller, "Thermal Rate Constant Calculation using Flux-Flux Autocorrelation Functions: Application to Cl + $H_2 \rightarrow$ HCl + H Reaction", J. Chem. Phys. **107**, 7194 (1997).
15. W.L. Hase, H. Wang, and G.H. Peslherbe, "Dynamics of Gas-Phase S_N2 Nucleophilic Substitution Reactions", in *Advances in Gas Phase Ion Chemistry*, Vol. 3, eds., L.M. Babcock and N.G. Adams, (JAI press, Greenwich, Connecticut, 1998).
16. T. Su, H. Wang, and W.L. Hase, "Trajectory Studies of S_N2 Nucleophilic Substitution. VII. F^- + $CH_3Cl \rightarrow FCH_3$ + Cl^-", J. Phys. Chem. A. **102**, 9819 (1998).

17. H. Wang, X. Sun, and W.H. Miller, "Semiclassical Approximations for the Calculation of Thermal Rate Constants for Chemical Reactions in Complex Molecular Systems", J. Chem. Phys. **108**, 9726 (1998).
18. H. Wang, W.H. Thompson, and W.H. Miller, " 'Direct' Calculation of Thermal Rate Constants for the F + H_2 $\rightarrow$ HF + H Reaction", J. Phys. Chem. A. **102**, 9372 (1998).
19. X. Sun, H. Wang, and W.H. Miller, "On the Semiclassical Description of Quantum Coherence in Thermal Rate Constants", J. Chem. Phys. **109**, 4190 (1998).
20. X. Sun, H. Wang, and W.H. Miller, "Semiclassical Theory of Electronically Nonadiabatic Dynamics: Results of a Linearized Approximation to the Initial Value Representation", J. Chem. Phys. **109**, 7064 (1998).
21. G.H. Peslherbe, H. Wang, and W.L. Hase, "Monte Carlo Sampling for Classical Trajectory Simulations", Adv. Chem. Phys. **105**, 171 (1999).
22. D. Lidar and H. Wang, "Calculating the Thermal Rate Constant with Exponential Speed-up on a Quantum Computer", Phys. Rev. E, **59**, 2429 (1999).
23. H. Wang, X. Song, D. Chandler, and W.H. Miller, "Semiclassical Study of Electronically Nonadiabatic Dynamics in the Condensed-Phase: Spin-Boson Problem with Debye Spectral Density", J. Chem. Phys., **110**, 4828 (1999).
24. H. Wang and W.H. Miller, "Analytic Continuation of Real-Time Correlation Function to Obtain Thermal Rate Constants for Chemical Reaction", Chem. Phys. Lett., **307**, 463 (1999).
25. H. Wang, M. Thoss, and W.H. Miller, "Forward-Backward Initial Value Representation for the Calculation of Thermal Rate Constants for Reactions in Complex Molecular System", J. Chem. Phys., **112**, 47 (2000).
26. R. Gelabert, X. Gimenez, M. Thoss, H. Wang, and W.H. Miller, "A Log-Derivative Formulation of the Prefactor for the Semiclassical Herman-Kluk Propagator", J. Phys. Chem. A. **104**, 10321 (2000).
27. H. Wang, "Basis Set Approach to the Quantum Dissipative Dynamics: Application of the Multi-Configuration Time-Dependent Hartree Method to the Spin-Boson Problem", J. Chem. Phys. **113**, 9948 (2000).
28. R. Gelabert, X. Gimenez, M. Thoss, H. Wang, and W.H. Miller, "Semiclassical Description of Diffraction and Its Quenching by the Forward-Backward Version of the Initial Value Representation", J. Chem. Phys. **114**, 2572 (2001).
29. H. Wang, M. Thoss, K. Sorge, R. Gelabert, X. Gimenez, and W.H. Miller, "Semiclassical Description of Quantum Coherence Effects and Their Quenching: A Forward-Backward Initial Value Representation Study", J. Chem. Phys. **114**, 2562 (2001).
30. M. Thoss, H. Wang, and W.H. Miller, "Generalized Forward-Backward Initial Value Representation for the Calculation of Correlation Functions in Complex Systems", J. Chem. Phys. **114**, 9220 (2001).
31. H. Wang, M. Thoss, and W.H. Miller, "Systematic Convergence in the Dynamical Hybrid Approach for Complex Systems: A Numerically Exact Methodology", J. Chem. Phys. **115**, 2979 (2001).
32. M. Thoss, H. Wang and W.H. Miller, "Self-Consistent Hybrid Approach for Complex Systems: Application to the Spin-Boson Model with Debye Spectral Density", J. Chem. Phys. **115**, 2991 (2001).
33. H. Wang, D.E. Manolopoulos, and W.H. Miller, "Generalized Filinov Transformation of the Semiclassical Initial Value Representation", J. Chem. Phys. **115**, 6317 (2001).
34. T. Yamamoto, H. Wang, and W.H. Miller, "Combining Semiclassical Time Evolution and Quantum Boltzmann Operator to Evaluate Reactive Flux Correlation Function for Thermal Rate Constants of Complex Systems", J. Chem. Phys. **116**, 7335 (2002).

35. M. Thoss and H. Wang, "Quantum Dynamical Simulation of Ultrafast Photoinduced Electron Transfer Processes in a Mixed-Valence Compound", Chem. Phys. Lett. **355**, 298 (2002).

36. H. Wang and M. Thoss, "Self-Consistent Hybrid Approach for Simulating Electron Transfer Reactions in Condensed Phases", Special issue on *Chemical Processes in Many-Body Quantum Systems*, Israel J. Chem., **42**, 167 (2002).

37. Y. Wang, W.L. Hase, and H. Wang, "Trajectory Studies of S_N2 Nucleophilic Substitution. IX. Microscopic Reaction Pathways and Kinetics for $Cl^- + CH_3Br$", J. Chem. Phys. **118**, 2688 (2003).

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39. H. Wang and M. Thoss, "Multilayer Formulation of the Multiconfiguration Time-Dependent Hartree Theory", J. Chem. Phys., **119**, 1289 (2003).

40. D. Egorova, M. Thoss, W. Domcke, and H. Wang, "Modeling of Ultrafast Electron-Transfer Processes: Validity of Multi-Level Redfield Theory", J. Chem. Phys., **119**, 2761 (2003).

41. M. Thoss, W.Domcke, and H. Wang, "Theoretical study of vibrational wave-packet dynamics in electron-transfer systems", Chem. Phys., **296**, 217 (2004).

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47. I. Kondov, H. Wang, and M. Thoss, "Theoretical Studies of Ultrafast Electron Transfer Reactions in Condensed Phases", *High Performance Computing in Science and Engineering, Munich 2004*, Eds., S. Wagner, W. Hanke, A. Bode and F. Durst, Springer (2005).

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50. H. Wang and M. Thoss, "Quantum mechanical evaluation of the Boltzmann operator in correlation functions for large molecular systems: a multilayer multi-configuration time-dependent Hartree approach", J. Chem. Phys., **124**, 034114 (2006).

51. I. Kondov, M. Thoss, and H. Wang, "Theoretical study of ultrafast heterogeneous electron transfer reactions at dye–semiconductor interfaces: Coumarin 343 at titanium oxide", J. Phys. Chem. A., **110**, 1364 (2006).

52. M. Thoss, I. Kondov, and H. Wang, "Quantum dynamics of ultrafast molecular processes in a condensed phase environment", in *Quantum Dynamics of Complex Molecular Systems*, *Springer Series in Chemical Physics , Vol. 83*, Eds. D. A. Micha and I. Burghardt, Springer (2006).

53. H. Wang, D. E. Skinner, and M. Thoss, "Calculation of reactive flux correlation functions for systems in a condensed phase environment: A multilayer multi-configuration time-dependent Hartree approach", J. Chem. Phys., **125**, 174502 (2006).

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56. I. Kondov, M. Cizek, C. Benesch, H. Wang, and M. Thoss, "Quantum dynamics of photoinduced electron-transfer reactions in dye–semiconductor systems: First principles description and application to coumarin 343–TiO_2", J. Phys. Chem. A, **111**, 11970 (2007).

57. I. R. Craig, M. Thoss, and H. Wang, "Proton transfer reactions in model condensed-phase environments: Accurate quantum dynamics using multilayer multiconfiguration time-dependent Hartree approach", J. Chem. Phys., **127**, 144503 (2007).

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65. H. Wang and M. Thoss, "From coherent motion to localization: Dynamics of the spin-boson model at zero temperature", *Focus issues: Quantum Dissipation in Unconventional Environments.* New J. Phys., **10**, 115005 (2008).

66. Y. Zhang, T. Irshaidat, H. X. Wang, K. V. Waynant, H. Wang, J. W. Herndon, "Coupling of Fischer carbene complexes with conjugated enediynes featuring radical traps; Novel structure and reactivity features of chromium complexed arene diradical species", J. Organometallic Chem. **693**, 3337 (2008).

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71. H. Wang and M. Thoss, "Numerically Exact Quantum Dynamics for Indistinguishable Particles: The Multilayer Multiconfiguration Time-Dependent Hartree Theory in Second Quantization Representation", J. Chem. Phys., **131**, 024114 (2009).

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73. H. Wang and M. Thoss, "From coherent motion to localization. II. Dynamics of the spin-boson model with sub-Ohmic spectral density at zero temperature", Chem. Phys., **370**, 78 (2010).

74. F. Ding, S. Chen, and H. Wang, "Computational Study of Ferrocene-Based Molecular Frameworks with 2,5-Diethynylpyridine as a Chemical Bridge", Materials, **3**, 2668 (2010).

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76. K. A. Velizhanin, M. Thoss, and H. Wang, "Meir-Wingreen formula for heat transport in a spin-boson nanojunction model", J. Chem. Phys., **133**, 084503 (2010).

77. J. Li, I. Kondov, H. Wang, and M. Thoss, "Theoretical Study of Photoinduced Electron Transfer Processes in the Dye-Semiconductor System Alizarin-TiO_2", J. Phys. Chem. C, **114**, 18481 (2010).

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92. Z. G. Yu, F. Ding, and H. Wang, "Hyperfine interaction and its effect on spin dynamics in organic solids", Phys. Rev. B, **87**, 205446 (2013).
93. E. Y. Wilner, H. Wang, G. Cohen, M. Thoss, and E. Rabani, "Bistability in a nonequilibrium quantum system with electron-phonon interactions", Phys. Rev. B, **88**, 045137 (2013).
94. V. Prucker, O. Rubio-Pons, M. Bockstedte, H. Wang, P. B. Coto, and M. Thoss, "Dynamical Simulation of Electron Transfer Processes in Alkanethiolate Self-Assembled Monolayers at the Au(111) Surface", J. Phys. Chem. C, **117**, 25334 (2013).
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100. L. Wei, H.-J. Wang, X. Chen, W. Fang, and H. Wang, "A comprehensive study of isomerization and protonation reactions in the photocycle of the photoactive yellow protein", Phys. Chem. Chem. Phys., **16**, 25263 (2014).
101. H. Wang, "Iterative Calculation of Energy Eigenstates Employing the Multilayer Multiconfiguration Time-Dependent Hartree Theory", J. Phys. Chem. A, **118**, 9253 (2014).
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105. Z. Tang, X. Ouyang, Z. Gong, H. Wang, J. Wu, "Extended hierarchy equation of motion for the spin-boson model", J. Chem. Phys., **143**, 224112 (2015).

Funded Research:

1. National Science Foundation-German Academic Exchange: "International: Quantum Dynamical Simulation of Ultrafast Electron Transfer Processes in Condensed Phases". Period: Feb.1, 2003 - Jan. 31, 2006. Amount: $6478.
2. American Chemical Society Petroleum Research Fund, Type G: "Quantum Dynamical Study of Ultrafast Photoinduced Electron Transfer Reactions in Mixed-Valence Systems". Period: Sept. 1, 2003 - Aug. 31, 2005. Amount: $35000.
3. National Science Foundation CAREER award: "Theoretical Study of Quantum Dynamics and Nonlinear Spectroscopy for Ultrafast Electron Transfer Processes in the Condensed Phase". Period: June 1, 2004 - May 31, 2010. Amount: $519362.
4. National Science Foundation, Collaborative Research in Chemistry (CRC): "Nanoparticle-mediated Electronic Communication", co-PI [with S. Chen (PI) and J.P. Konopelski (co-PI) of UC Santa Cruz]. Period: September 15, 2008 - September 14, 2010. Amount: $660,000 (NMSU Share: $148,998).
5. LANL-MOU: "Quantum Dynamics Study of Enzymatic and Non-enzymatic Hydrolysis Reactions", PI [with I. Vasiliev (co-PI, NMSU), A. Piriyatinsky (co-PI, LANL), T.C. Germann (co-PI, LANL)]. Period: August 1, 2008 - September 30, 2010. Amount: $67,500.
6. National Science Foundation: "Quantum Dynamics Study of Ultrafast Electron Transfer Reactions". Period: September 1, 2010 - August 31, 2013. Amount: $405,000.
7. National Science Foundation: "Developing the multilayer multiconfiguration time-dependent Hartree theory". Period: July 1, 2014 - June 31, 2017. Amount: $420,000.