

## CURRICULUM VITAE

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**5. Publications:**

1. W. P. Reinhardt and J. D. Doll, "Direct Calculation of Natural Orbitals by Many-Body Perturbation Theory: Application to Helium", J. Chem. Phys, **50**, 2767 (1969).
2. J. D. Doll, " Many-Body Green's Function Theory: Atomic and Molecular Applications", Harvard Thesis, 1971.

3. J. D. Doll and W. P. Reinhardt, " Many-Body Green's Functions for Finite, Non-Uniform Systems: Applications to Closed Shell Atoms", J. Chem. Phys. **57**, 1169 (1972).
4. J. D. Doll and W. H. Miller, " Classical Limit Quantization of Non-Separable Systems: Multi-Dimensional WKB Perturbation Theory", J. Chem. Phys. **57**, 4428 (1972).
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11. J. D. Doll, " Semiclassical Theory of Atom-Solid Surface Collisions: Elastic Scattering", Chem. Phys. **3**, 257 (1974).
12. J. D. Doll, "Semiclassical Theory of Atom-Solid Surface Collisions: Application of He/LiF Diffraction," J. Chem. Phys. **61**, 954 (1974).

13. J. D. Doll, " Determination of Gas/Surface Interaction Potentials: Extraction of the Lennard-Jones, Devonshire Strength Parameter", Chem. Phys. Letts. **29**, 195 (1974).
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16. J. D. Doll, L. E. Myers and S. A. Adelman, "Generalized Langevin Equation Approach for Atom/Solid-Surface Scattering: Inelastic Studies", J. Chem. Phys. **63** 4908 (1975).
17. J. D. Doll and D. Dion, "Brownian Dynamics for Gaussian Random Sources", Chem. Phys. Letts. **37**, 386 (1976).
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19. S. A. Adelman and J. D. Doll, " Generalized Langevin Equation Approach for Atom/Solid-Surface Scattering: General Formalism for Classical Scattering off Harmonic Solids", J. Chem. Phys. **65**, 2375 (1976).
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141. Art E. Cho, J. D. Doll, and D. L. Freeman, "Wavelet Formulation of Path Integral Monte Carlo," *J. Chem. Phys.* **117**, 5971 (2002).
142. Markus Meuwly and J. D. Doll, "Dynamical Studies of Mixed Rare Gas Clusters: Collision Induced Absorption in  $(\text{Ne})_n (\text{Ar})_m$  ( $n + m \leq 30$ )," *Phys. Rev. A* **66**, 023202 (2002).

143. Cristian Predescu and J. D. Doll, "Optimal Series Representations for Numerical Path Integral Simulations," *J. Chem. Phys.* **117**, 7448 (2002).
144. Cristian Predescu and J. D. Doll, "Random Series and Discrete Path Integral methods: The Levy-Ciesielski Implementation," *Phys. Rev. E*, **67**, 026124 (2003).
145. Dubravko Sabo, D. L. Freeman, and J. D. Doll, "Taming the Rugged Landscape: Techniques for the Production, Reordering and Stabilization of Selected Cluster Inherent Structures," *J. Chem. Phys.* **118**, 7321 (2003).
146. C. Predescu, D. Sabo, and J. D. Doll, "Numerical Implementation of Some Reweighted Path Integral Methods," *J. Chem. Phys.* **119** 4641 (2003).
147. Cristian Predescu, Dubravko Sabo, David L. Freeman, and J. D. Doll, "Energy Estimators for Random Series Path Integral Methods," *J. Chem. Phys.* **119**, 10475 (2003).
148. Cristian Predescu, Dubravko Sabo, David L. Freeman and J. D. Doll, "Heat Capacity Estimators for Random Series Path-integral Methods by Finite-difference Schemes," *J. Chem. Phys.* **119** 12119 (2003).
149. G. Guralnik, J. D. Doll, R. Easther, P. Emirdag, D. D. Ferrante, S. Hahn, D. Petrov, and D. Sabo, "Alternative numerical techniques," *Nucl. Phys. B. Proc. Sup.* **119** 950 (2003).
150. D. D. Ferrante, J. Doll, G. Guralnik, and D. Sabo, "Mollified Monte Carlo," *Nucl. Phys. B. Proc. Sup.* **119** 965 (2003).
151. Cristian Predescu, J. D. Doll, "Short Review of Recent Developments for Path-Integral Techniques: Monte Carlo Methods for Real Time Integration," in *The Monte Carlo Method in the Physical Sciences*, J. Gubernatis, ed., (American Institute of Physics Conference Proceedings, volume 690, Melville, NY (2003)), 269-280.
152. Dubravko Sabo, J.D.Doll and David L. Freeman, "Monte Carlo Methods for Real Time Integration," in *The Monte Carlo Method in the Physical Sciences*, J. Gubernatis, ed., (American Institute of Physics Conference Proceedings, volume 690, Melville, NY (2003)), 396-397.

153. Cristian V. Diaconu, Art E. Cho, J. D. Doll, and David L. Freeman, "Broken Symmetry Unrestricted Hybrid Density Functional Calculations on Nickel Dimer and Nickel Hydride," *J. Chem Phys.* **121** 10026 (2004).
154. Pablo Nigra, D. L. Freeman, Dubravko Sabo, J. D. Doll, "On the Encapsulation of Nickel Clusters by Molecular Nitrogen," *J. Chem. Phys.* **121** 475 (2004).
155. Dubravko Sabo, Cristian Predescu, J. D. Doll and D. L. Freeman, "Phase Changes in Selected Lennard-Jones  $X_{13-n}Y_n$  Clusters," *J. Chem. Phys.* **121** 856 (2004).
156. Dubravko Sabo, D. L. Freeman and J. D. Doll, "Taming the Rugged Landscape: Production, Reordering and Stabilization of Selected Cluster Inherent Structures in the AnB13-n System," *J. Chem. Phys.* **121** 847 (2004).
157. J. Doll, "A Modern Perspective on Transition State Theory," in *Encyclopedia of Materials Modeling. Volume One, Fundamental Models and Methods*, S. Yip and H. Metiu, eds, (MIT Press, Cambridge, 2005).
158. Pablo Nigra, David L. Freeman, and J. D. Doll, "Combining Smart Darting with Parallel Tempering using Eckart Space: Application to Lennard-Jones Clusters," *J. Chem. Phys.* **122** 114113 (2005).
159. Dubravko Sabo, David L. Freeman and J. D. Doll, "Pressure Dependent Study of the Solid-solid Phase Change in LJ38," *J. Chem. Phys.* **122** 094716 (2005).
160. Stephen F. Langley, E. Curotto, D. L. Freeman, and J. D. Doll, "Rigid quantum Monte Carlo simulations of condensed molecular matter: Water clusters in the  $n = 2 - 8$  range," *J. Chem. Phys.* **126**, 084506 (2007).
161. Dubravko Sabo, Markus Meuwly David L. Freeman, J. D. Doll, "A Constant Entropy Increase Model for the Selection of Parallel Tempering Ensembles," *J. Chem. Phys.* **128**, 174109 (2008).
162. E. Curotto, D. L. Freeman, J. D. Doll, "A stereographic projection path integral study of the coupling between the orientation and the bending degrees of freedom of water," *J. Chem. Phys.* **128** 204107 (2008).
163. Nuria Plattner, Tobias Bandi, J. D. Doll, David L. Freeman and Markus Meuwly, "MD Simulations using Distributed Multipole Electrostatics: Structural and



Spectroscopic Properties of CO- and Methane-Containing Clathrates," *Mol. Phys.* **106** 1675 (2008).

164. Sharif Kunikeev, David L. Freeman, and J.D. Doll, "A Numerical Study of the Asymptotic Convergence Characteristics of Partial Averaged and Reweighted Fourier Path Integral Methods," *Int. J. Quantum Chemistry* **109** 2916 (2009).
165. E. Asare, A. Musah, E. Curotto, David L. Freeman, and J. D. Doll, "The Thermodynamic and Ground State Properties of the TIP4P Water Octamer," *J. Chem. Phys.* **131** 184508 (2009).
166. J. D. Doll, J. E. Gubernatis, Nuria Plattner, Markus Meuwly, P. Dupuis, H. Wang, "A Spatial Averaging Approach to Rare-Event Sampling," *J. Chem. Phys.* **131**, 104107 (2009).
167. Nuria Plattner, J. D. Doll, and Markus Meuwly, "Spatial Averaging Applied to Small Molecule Diffusion in Condensed Phase Environments," *J. Chem. Phys.* **133** 044506 (2010).
168. Markus Meuwly and J. D. Doll, "Finite Temperature Quantum Simulations of Mixed Rare Gas Clusters," *J. Chem. Phys.* **132** 234315 (2010).
169. Sharif D. Kunikeev, David L. Freeman and J.D. Doll, "Convergence Characteristics of the Cumulant Expansion for Fourier Path Integrals," *Phys. Rev. E*, **81**, 066707 (2010).
170. B. M. Rubenstein, J. E. Gubernatis, and J. D. Doll, "Comparative Monte Carlo Efficiency by Monte Carlo Analysis," *Phys. Rev. E*, **82**, 036701 (2010).
171. Nuria Plattner, Sharif Kunikeev, David L. Freeman, and J.D. Doll, "Numerical Investigation of the Cumulant Expansion for Fourier Path Integrals," Reykjavik Para2010 Conference Proceedings (Springer-in press).

#### **Invited Lectures and Papers Read:**

"Quantum Monte Carlo Dynamics", an invited talk presented at the Lake Arrowhead Conference on The Role of Nonlinear Dynamics in Reaction Kinetics, Lake Arrowhead, CA March 7-9, 1988.

"Quantum Monte Carlo Dynamics", an invited talk presented to the national American Physical Society Meeting, New Orleans, March 24, 1988.

"Randomly Exact Methods: New Tools in Theoretical Chemistry", Department of Chemistry, University of Wisconsin, Madison, Wisconsin, August 16, 1988.

"Recent Developments in Real Time Path Integral Methods", Simulation Physics Working Group, Los Alamos National Laboratory, Los Alamos, NM September 6, 1988.

"Randomly Exact Methods: New Tools in Theoretical Chemistry", Department of Chemistry, Brown University, Providence, RI, September 9, 1988.

"Theoretical Studies of Time Correlation Functions", Divisional Review Presentations, Los Alamos National Laboratory, Los Alamos, NM, September 21, 1988.

"Monte Carlo Theory: Plain and Fancy", an invited talk at the University of Texas Conference on Supercomputing, October 5, 1988.

"Monte Carlo Methods in Chemistry", Departmental Colloquium, Department of Chemistry, University of Michigan, January 10, 1989.

"Randomly Exact Methods", an invited talk presented at the AAAS national meeting, San Francisco, January 17, 1989.

"Monte Carlo Methods in Chemistry", UC Irvine Institute for Surface and Interface Science Workshop on Molecular Dynamics, Irvine, CA, March 9, 1989.

"Randomly Exact Methods", invited seminar, Department of Chemistry, University of Missouri, Columbia, Missouri, March 31, 1989.

"A Random Approach to Time", invited paper, Sanibel Symposium on Theoretical Chemistry and Biology, University of Florida, held at St. Augustine, Florida, April 6, 1989.

"Recent Developments in Surface Diffusion", invited talk, Division of Colloid and Interface Science, Dallas ACS meeting, Dallas, Texas, April 11, 1989.

"Cluster Melting", invited talk, Division of Physical Chemistry, Dallas ACS meeting, Dallas, Texas, April 11, 1989.

"Quantum Monte Carlo Dynamics", invited talk, Division of Physical Chemistry, Miami ACS meeting, Miami Beach, September 14, 1989.

"Recent Developments in the Theory of Surface Diffusion", Department of Physics, Brown University, October 5, 1989.

"Quantum Dynamical Implications of Chaco Canyon", Department of Chemistry, Brown University, October 19, 1989.

"Quantum Monte Carlo Dynamics", Department of Chemistry, Columbia University, February 22, 1990.

"The Quantum Mechanics of Clusters: Dynamics of Rare Gas Systems", Department of Chemistry, University of Pennsylvania, March 9, 1990.

"The Quantum Dynamics of Clusters", Los Alamos National Laboratory, Los Alamos, NM, July 26, 1990.

"The Quantum Dynamics of Clusters", American Conference on Theoretical Chemistry, San Diego, August 2, 1990.

"The Quantum Dynamics of Clusters", Invited Talk, American Chemical Society National Meeting, Washington, DC, August 28, 1990.

"The Quantum Dynamics of Clusters", Department of Chemistry, Boston University, October 29, 1990.

"The Quantum Dynamics of Clusters", Department of Chemistry, University of Massachusetts, Amherst, November 6, 1990.

"The Quantum Dynamics of Clusters", Canadian Conference on Computational Chemistry, Orford, Canada, May 19-23, 1991.

"The Quantum Dynamics of Clusters", Computer Simulations in Chemical Physics: Recent Advances and New Directions, Irvine, CA, June 24-28, 1991.

"The Quantum Dynamics of Adsorbates," Dynamics of Gas-Surface Interactions Gordon Conference, Andover, NH, August 8, 1991.

"Quantum Monte Carlo Dynamics," Los Alamos, NM, November 25, 1991.

"Quantum Monte Carlo Dynamics," University of Illinois, Chicago, March 19, 1992.

"The Quantum Dynamics of Hydrogen Adsorbates," Telluride Research Conference, July 15, 1992.

"The Quantum Dynamics of Hydrogen Adsorbates," ACS Meeting, August 24, 1992.

"The Quantum Dynamics of Hydrogen Adsorbates," Department of Chemistry, Boston College, October 15, 1992.

“Quantum Monte Carlo Dynamics,” Theoretical Physics Group, Brown University, December 14, 1992.

“The Interfacial Dynamics of Metal/Hydrogen Systems,” Department of Chemistry, Queens College, New York, February 17, 1993.

“The Interfacial Dynamics of Metal/Hydrogen Systems,” American Physical Society meeting, Seattle, March 23, 1993.

“The Quantum Dynamics of Adsorbates,” American Chemical Society national meeting, Denver, April 1, 1993.

“Monte Carlo Methods in Chemistry,” Brown University Computer Science Department, April 15, 1993.

“Dynamics of Interfacial Hydrogen,” Workshop on Interfacial Phenomena, Copenhagen, May 1993.

“Dynamics of Interfacial Hydrogen,” American Conference on Theoretical Chemistry, Rochester,

June 1993.

“Dynamics of Interfacial Hydrogen,” Gordon Conference on Surface Science, Andover, NH, August 1993

“Dynamics of Interfacial Hydrogen,” Surface Chemistry Group, Brown University, November 1993

“Randomly Exact Methods,” Undergraduate Physics Seminar, Department of Physics, Brown University, November 1993

“Dynamics of Interfacial Hydrogen,” Department of Chemistry, Wesleyan University, January 21, 1994.

“Dynamics of Interfacial Hydrogen,” Department of Chemistry, University of Maryland, February 12, 1994.

“Dynamics of Interfacial Hydrogen,” University of New Hampshire, February 24, 1994.

“Dynamics of Interfacial Hydrogen,” Department of Chemistry, SUNY Stony Brook, March 10, 1994.

“Dynamics of Interfacial Hydrogen,” University of Colorado, March 18, 1994.

“Bayesian Dynamics,” Los Alamos National Laboratory, March 21, 1994.

“The Structure of Quantum Dynamics,” Telluride Conference on Quantum Dynamics, July 18, 1994.

“Dynamics of Interfacial Hydrogen,” New York University, Chemistry, October 21, 1994.

“Dynamics of Interfacial Hydrogen,” Princeton University, Chemistry, November 10, 1994.

“The Structure of Quantum Dynamics,” Los Alamos Conference on Quantum Dynamics, January 10-13, 1995.

“Asynchronous Learning Networks in Chemistry”, A. P. Sloan Foundation, New York, March 17, 1995.

“Dynamics of Interfacial Hydrogen,” University of New Hampshire, Chemistry, May 11, 1995.

“If Newton had Owned a Mac,” University Lecture, Brown University, November 9, 1995.

“Asynchronous Learning Networks in Chemistry”, NERCOMP Conference, Providence, April 2, 1996.

“Asynchronous Learning Networks in Chemistry”, Center for the Advancement of College Teaching, Providence, April 10, 1996.

“Asynchronous Learning Networks in Chemistry”, A. P. Sloan Foundation Workshop on Asynchronous Learning Networks, Urbana, May 3-4, 1996.

“Embedded Cluster Approach to Quantum Dynamics,” Gordon Conference on Few Particle Dynamics, Andover, NH, August 11-16, 1996.

“Path Integral and Quantum Monte Carlo Studies of Metal/Hydrogen Clusters,” Second International Symposium on Theory of Atomic and Molecular Clusters, Lake Geneva, Wisconsin, September 15-20, 1996.

“The Quantum Mechanics of Interfacial Hydrogen in Metals,” Los Alamo Physics Colloquium, Los Alamos, New Mexico, September 26, 1996.

“The Quantum Mechanics of Interfacial Hydrogen in Metals,” Department of Chemistry, Southern Methodist University, Dallas, Texas, October 7, 1996.

“The Quantum Mechanics of Interfacial Hydrogen in Metals,” Department of Chemistry, University of Texas at Arlington, Arlington, Texas, October 8, 1996.

“The Quantum Mechanics of Interfacial Hydrogen in Metals,” Southwest Theoretical Chemistry Conference, Arlington, Texas, November 15, 1996.

“Recent Developments in Quantum Dynamics,” Center for Non-linear Studies, Los Alamos National Lab, December 18, 1996.

“The Quantum Mechanics of Interfacial Hydrogen in Metals: An Introduction,” Enrico Fermi Summer School on Rare Event Dynamics, Lerici, Italy, July 11, 1997.

“Real Time Quantum Dynamics,” Frontiers of Monte Carlo Methods Conference, Los Alamos, NM, January 15, 1998.

“The Quantum Mechanics of Interfacial Hydrogen in Metals,” Department of Chemistry, University of Michigan, Ann Arbor, MI, January 29, 1998.

“Real Time Quantum Dynamics,” Invited Lecturer, CECAM Path Integral Conference, Turin, Italy, June, 1998.

“Real Time Quantum Dynamics,” Invited Lecturer, NATO Advanced Study Institute: Quantum Monte Carlo methods in chemistry and physics, Cornell University, Ithaca, NY, July, 1998.

“Asynchronous Learning Networks in Chemistry,” Department of Chemistry, University of Kansas, Lawrence, Kansas, October, 1998.

“The Quantum Mechanics of Interfacial Hydrogen in Metals,” Department of Chemistry, University of Kansas, Lawrence, Kansas, October, 1998.

“The Quantum Mechanics of Interfacial Hydrogen in Metals,” Brian Head Workshop on Quantum Dynamics, Brian Head, UT, March 13-18, 1999.

“Dimensional Strategies and the Minimization Problem: Barrier Avoiding Algorithms,” Atomic and Molecular Theory Group, Los Alamos National Laboratory, August, 1999

“The Quantum Mechanics of Interfacial Hydrogen in Metals,” Department of Chemistry, Boston University, March 29, 2000.

“The Quantum Mechanics of Interfacial Hydrogen in Metals,” Department of Chemistry, University of Massachusetts, April 13, 2000.

“The Quantum Mechanics of Interfacial Hydrogen in Metals,” CECAM Workshop on Long-Time Dynamics, Reykyavik, Iceland, 23-30 June 2000.

“Dynamical Inherent Structures,” Pacificchem 2000, International Chemical Congress of Pacific Basin Societies (invited talk), Honolulu, 14-19 December 2000.

“Equilibrium and Dynamical Inherent Structures: A Probabilistic Approach,” San Diego ACS National Meeting (invited talk), 31 March-2 April 2001.

“Quantum Monte Carlo Dynamics,” Chicago ACS Meeting (invited talk), August 2001.

“Structure and Dynamics of Hydrogen in Metals,” Chemistry, University of Iceland, Reykjavik September 2001.

“Stochastic Methods for the Complex Quadrature Problem,” Physics, University of Iceland, Reykjavik, September 2001.

“Randomly Exact Methods: Monte Carlo Methods in Chemistry,” Department of Chemistry, Georgia Tech, 29 November 2001.

“Randomly Exact Methods: Monte Carlo Methods in Chemistry,” Department of Chemistry, Emory University, 30 November 2001.

“Randomly Exact Methods: Monte Carlo Methods in Chemistry,” Society of Undergraduate Mathematics, Brown University, Providence, RI, April 2002.

“Dynamical Inherent Structures: Long-time Quantum Dynamics,” International Conference on Clusters and Nanotechnology (invited talk), San Juan, Puerto Rico, April 2002.

“Randomly Exact Methods: Monte Carlo Methods in Chemistry,” King Faud’s Visiting Students, Brown University, Providence, RI, May 2002.

“Randomly Exact Methods: Monte Carlo Methods in Chemistry,” Gordon Summer School (series of 3 invited lectures), Bristol, RI, June 2002.

“Dimensionality as a Tool in Simulation,” Bio-Med Department, Brown University, April 2003.

“Dynamical Path Integral Methods,” Metropolis 50th Anniversary Workshop, Los Alamos, June 2003 (invited talk).

“The Structure and Dynamics of Clusters: Concepts, Tools and Applications,” Departments of Physics and Chemistry, University of Nevada, Reno, October 9, 2003.

“The Structure and Dynamics of Clusters: Concepts, Tools and Applications,” University of New Orleans, November 14, 2003.

“The Structure and Dynamics of Clusters: Concepts, Tools and Applications,” University of New Orleans, November 14, 2003.

“The Structure and Dynamics of Clusters: Concepts, Tools and Applications,” Departments of Physics and Center for Materials for Information Technology, University of Alabama, March 11, 2004.

“Dimensionality: It Ain’t What it Used to Be,” Department of Physics, Brown University, March 31, 2004.

“Structure & Dynamics of Many-Body Systems: Concepts, Tools and Applications.,” Brown University Briefing to Oak Ridge National Laboratory Officials, May 10, 2004.

“Structure & Dynamics of Many-Body Systems: Concepts, Tools and Applications.,” Mercury Conference, Hamilton College, Clinton, NY, July 29, 2004.

“Recent Developments in Path-Integral Monte Carlo,” Joint Harvard/MIT/BU Chemistry Seminar, September 22, 2004.

June 26-July 2, 2005, Presented a series of three invited lectures on classical and quantum-Monte Carlo methods at the Utah ACS Summer School.

“Stochastic Methods in Chemistry,” September 11-13, 2006, Swiss National Computing Center, Manno Switzerland. A series of 4 invited talks.

“Stochastic Methods in Chemistry,” August 2007, Canadian Conference on Theoretical Chemistry, St. John’s Newfoundland (invited talk).

“The Long Way Home,” August 2008, Workshop on Advances in Chemical Dynamics (organized in my honor), Sante Fe. NM.

“Robin Hood and the Rare-Event Problem: Recent Developments in Monte Carlo Methods,” Department of Chemistry, University of Kansas, April 30, 2009.

“Robin Hood and the Rare-Event Problem: Recent Developments in Monte Carlo Methods,” Department of Chemistry, University of Missouri, May 1, 2009.

"Recent Developments in Rare-Event Monte Carlo Methods," , Department of Chemistry, Dartmouth College, May 6, 2010.

"Recent Developments in Rare-Event Monte Carlo Methods," , Para2010 Conference on Parallel Computing, Reykjavik Iceland, June 6, 2010.

**6. Research in progress:**

Equilibrium and dynamical studies of many-body systems.

Theory of stochastic processes.

Classical and quantum Monte Carlo methods.

Real time quantum Monte Carlo methods.

The study of condensed matter, especially the study of solid surfaces and clusters.



7. **Service:**

**i) To the University:**

**ii)** Provost's Committee on the Future of Academic Computing (2003-2009)

**iii)** Faculty Advisory Committee, CCV, Brown University (2002-2009)  
Hybrid Supercomputer Advisory Committee,  
Brown University (1989)  
Faculty Liaison - baseball team, 1991, 1992  
Faculty Liaison - DUG, 1992  
Graduate Admissions Committee, 1992, 1993, 1994, 1995, 1996, 1997  
Computer Committee, 1997, 1998, 1999, 2000  
Recruiting Committee, 1997  
\*Research Proposal committees for Ryu and Ma, November 1999

**iv) To the Profession:**

Member DOE ASCI Review Panel, University of Utah, September 2002.  
Member of AFOSR Chemical Dynamics Review Panel, Boston, May 24-25, 2000. \*Member of LDRD Review Panel, Los Alamos National Laboratory, Los Alamos, NM, August 1999.  
\*Member AFOSR Chemical Dynamics Review Panel, Washington, DC, June 2-3, 1999  
Member, DOE ASCI Utah Review team, Salt Lake City, UT, October, 1998  
Invited Lecturer, NATO Summer School on Quantum Monte Carlo Methods, Cornell, July, 1998.  
Invited Lecturer, CECAM workshop on Quantum Monte Carlo Methods, Turin, Italy, June 1998.  
Co-Organizer, Frontiers of Monte Carlo Methods Conference, Los Alamos, January, 1998.  
Member of Department of Energy's External Lawrence Berkeley Laboratory Chemical Sciences Review Panel, March 1997.  
Invited Lecturer, Enrico Fermi Summer School, Lerici, Italy, July, 1997.  
Member of Department of Energy's External Review Panel, Argonne national Laboratory, Metal Clusters Program, November, 1997.  
Co-organized Conference on Monte Carlo Methods for the 21st Century, Los Alamos, January, 1998

**v) Service (cont'd)**

Member, Executive Panel, Division of Physical Chemistry  
ACS (1990-1993)  
Co-organizer of the ACS symposium on New Frontiers in  
Electronic Structure and Dynamics, August 1990.  
Co-organizer of the Quantum Simulations of Condensed Matter  
Conference, Los Alamos, 1989  
Member National Science Foundation Science and Technology  
Center Advisory Panel, 1988.  
Co-organizer Metropolis Quantum Monte Carlo conference,  
Los Alamos, 1985  
Co-organizer CECAM meeting on condensed-phase reaction dynamics, Purdue, 1984.  
Member of Air Force Office of Scientific Research Chemistry Panel, 1983-1986.  
Co-organizer CECAM meeting on surface chemistry, New Platz, 1982  
Member of DOE panel on surface physics, 1977  
Member of NSF panel on lasers in chemistry, 1975

**8. Academic Honors:**

Department Awards in Chemistry, University of Kansas  
(1964, 1966, 1967).  
Departmental Award in German, University of Kansas (1967).  
B.S. Chemistry, With highest distinction, University of  
Kansas (1967).  
Phi Lambda Upsilon, University of Kansas (1967).  
Phi Beta Kappa, University of Kansas (1967).  
Federal Republic of Germany, Graduate Exchange Fellowship  
(DAAD, 1967) - declined  
National Science Foundation Predoctoral Fellow,  
Harvard (1967-1971).  
Outstanding Teaching Fellow Award, Harvard (1971).  
National Science Foundation Postdoctoral Fellow,  
Berkeley (1971-1972).  
Alfred P. Sloan Fellow (1976-1978).  
Selection as Laboratory Fellow, Los Alamos National  
Laboratory (1981).  
Distinguished Visiting Lecturer, University of Texas (1983).  
Selected by *Science Digest* as one of America's 100 Brightest  
Scientists Under Age 40 (1984)  
Named the Jesse H. and Louisa D. Sharpe Metcalf Professor of Chemistry (1995)

**Current Grants:**

“Large Deviation Methods for the Analysis and Design of Monte Carlo Schemes in Physics and Chemistry,” DOE, (Brown Portion: \$758,659, Los Alamos Portion: \$513,358), 1/01/09 – 12/31/11). Co-PI with P. Dupuis and H. Wang (Applied Math, Brown) and J. Gubernatis (Los Alamos).

### **Academic Honors (cont'd)**

“Workstation Network for Computational Physics and Chemistry in Rhode Island,” NSF-CHE 9203498: 7/1/92 - 1/31/94, \$ 285,617 (including institutional matching funds).

“Chemical Information Preprint System,” Camille and Henry Dreyfus Foundation, \$15,000, 11/1/93 - 10/31/95.

“Asynchronous Learning Networks in Chemistry,” A. P. Sloan Foundation, \$ 29,800, October 1, 1994 - April 30, 1995.

“Equilibrium and Dynamics of Many Body Systems: Near Surface Hydrogen in Transition Metals,” NSF: CHE 9411000, \$558,000, November 1, 1994 - October 31, 1997.

“Integrated Learning Networks in Chemical Education,” Sloan Foundation, \$248,000, July 1, 1995 - June 30, 1999.

“Information Systems for Chemical Research and Education,” National Science Foundation, NSF Grant CHE-9523287. \$23,906 (August 1, 1995 - July 31, 1996).

“The Rhode Island Workstation Network for Computational Chemistry and Physics,” NSF Grant 9625498. \$246,000 (including institutional matching funds), 8/1/96 - 7/31/98.

“Acquisition of a CAVE and a Shared-Memory Supercomputer,” NSF Major Research Instrumentation Program CDA-9724347, \$1,361,225, 11/1/97 - 10/31/99 (including institutional matching funds, joint with several Brown University faculty).

“The Influence of Adsorbate-Adsorbate Interactions on the Dynamics of Interfacial Hydrogen,” NSF CHE-9714970, \$601,500, 11/1/97 - 10/31/2001.

“Asynchronous Learning Networks at Brown,” Davis Foundation, \$ 250,000, 6/1/98-5/31/2000.

### **9. Courses taught:**

Year	Fall, Spring Semester
1989-90	Chemistry 277, 278
1990-91	Chemistry 31, 278
1991-92	Chemistry 31, 278
1992-93	Chemistry 31, 278
1993-94	Chemistry 31, 278

1994-95	Chemistry 31, 278
1995-96	Chemistry 31, 278
1997-98	Chemistry 21 (all sections), no teaching semester ii
1998-99	Chemistry 21 (all sections), no teaching semester ii
1999-00	Chemistry 21 (all sections), no teaching semester ii
2000-01	Chemistry 156, Chemistry 115
2001-02	Sabbatical Semester, Chemistry 115
2002-03	Chemistry 114, Chemistry 115
2003-04	Chemistry 114, Chemistry 115
2004-05	Chemistry 114, Chemistry 115
2005-06	Chemistry 33, Chemistry 115
2006-07	Chemistry 33, Chemistry 202
2007-08	Chemistry 33, Chemistry 202
2008-09	On leave, Chemistry 202
2009-10	Chemistry 114, Chemistry 115
2010-11	Chemistry 277, Chemistry 278

**Current Research Group:**

Nuria Plattner      Postdoctoral Fellow (Swiss National Science Foundation, 2010-)

**10. CV Updated: 14 January 2011**