

*Curriculum Vitae*

**KATHARINE CLARKE HUNT**

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**Experience**

10/92-present     University Distinguished Professor, Department of Chemistry,  
Michigan State University, East Lansing, Michigan

10/98-8/02        Chairperson, Department of Chemistry,  
Michigan State University

7/89 -9/92        Professor of Chemistry, Michigan State University

7/84 - 6/89        Associate Professor of Chemistry, Michigan State University

9/79 - 6/84        Assistant Professor of Chemistry, Michigan State University

10/78 - 9/79      National Science Foundation Postdoctoral Fellow  
Massachusetts Institute of Technology  
Cambridge, Massachusetts  
Research advisor: Professor John Ross

**Education**

Ph.D.              Theoretical Chemistry, September 1978  
University of Cambridge, England  
Research advisor: Professor A. D. Buckingham

B.S.                Chemistry, June 1975  
Michigan State University

**Honors and Awards**

National Science Foundation National Needs Postdoctoral Fellowship, 1978-79  
Marshall Scholarship, 1975-78  
Danforth Fellowship, 1975-78  
MSU Board of Trustees Award, 1975  
Michigan State University Alumni Distinguished Scholarship, 1971-75  
National Merit Scholarship, 1971-75  
Phi Beta Kappa  
Phi Kappa Phi  
Sigma Xi  
    MSU Sigma Xi Junior Research Award, 1991  
    MSU Sigma Xi Senior Research Award, 2001  
International Conference of Computational Methods in Sciences and Engineering  
(ICCMSE), Distinguished Career Prize, 2009  
Norman L. and Olga K. Fritz Excellence in Teaching Award, College of Natural Science, 2020

## Publications

1. K. L. Clarke, P. A. Madden, and A. D. Buckingham, Collision-induced polarizabilities of inert gas atoms, *Mol. Phys.* **36**, 301-16 (1978).
2. A. D. Buckingham and K. L. Clarke, Long-range effects of molecular interactions on the polarizability of atoms, *Chem. Phys. Lett.* **57**, 321-25 (1978).
3. K. L. Clarke Hunt and A. D. Buckingham, The polarizability of H<sub>2</sub> in the triplet state, *J. Chem. Phys.* **72**, 2832-40 (1980).
4. A. D. Buckingham and K. L. Clarke Hunt, The pair polarizability anisotropy of SF<sub>6</sub> in the point-atom-polarizability approximation, *Mol. Phys.* **40**, 643-48 (1980).
5. K. L. C. Hunt, Long-range dipoles, quadrupoles, and hyperpolarizabilities of interacting inert-gas atoms, *Chem. Phys. Lett.* **70**, 336-42 (1980).
6. Katharine L. C. Hunt and John Ross, Path integral solutions of stochastic equations for nonlinear irreversible processes: The uniqueness of the thermodynamic Lagrangian, *J. Chem. Phys.* **75**, 976-84 (1981).
7. K. L. C. Hunt, B. A. Zilles, and J. E. Bohr, Effects of van der Waals interactions on the polarizability of atoms, oscillators, and dipolar rotors at long range, *J. Chem. Phys.* **75**, 3079-86 (1981).
8. K. L. C. Hunt, Nonlocal polarizability densities and van der Waals interactions, *J. Chem. Phys.* **78**, 6149-55 (1983).
9. Paul M. Hunt, Katharine L. C. Hunt, and John Ross, Path integral solutions for Fokker-Planck conditional propagators in nonequilibrium systems: Catastrophic divergences of the Onsager-Machlup-Laplace approximation, *J. Chem. Phys.* **79**, 3765-72 (1983).
10. K. L. C. Hunt, Nonlocal polarizability densities and the effects of short-range interactions on molecular dipoles, quadrupoles, and polarizabilities, *J. Chem. Phys.* **80**, 393-407 (1984).
11. J. Kottalam and K. L. C. Hunt, Numerical studies of fluctuations and hysteresis in the homogeneous Schlögl model, in *Fluctuations and Sensitivity in Nonequilibrium Systems*, edited by W. Horsthemke and D. K. Kondepudi (Springer-Verlag, New York, 1984), 242-44.
12. Katharine L. C. Hunt, *Ab initio* and approximate calculations of collision-induced polarizabilities, in *Phenomena Induced by Intermolecular Interactions*, edited by G. Birnbaum, NATO ASI Ser. B **127** (Plenum, New York, 1985), 263-90.
13. Katharine L. C. Hunt, Classical multipole models: Comparison with *ab initio* and experimental results, in *Phenomena Induced by Intermolecular Interactions*, edited by G. Birnbaum, NATO ASI Ser. B **127** (Plenum, New York, 1985), 1-28.
14. K. L. C. Hunt and J. E. Bohr, Effects of van der Waals interactions on molecular dipole moments: The role of field-induced fluctuation correlations, *J. Chem. Phys.* **83**, 5198-202 (1985).
15. Katharine L. C. Hunt, Paul M. Hunt, and John Ross, Path integral methods in nonequilibrium chemical thermodynamics: Numerical tests of the Onsager-Machlup-Laplace approximation and analytic continuation techniques, in *Path Integrals from meV to MeV*, edited by M. C. Gutzwiller, A. Inomata, J. R. Klauder, and L. Streit (World Scientific, 1986), 199-216.
16. J. Juanós i Timoneda and K. L. C. Hunt, Label-free exchange perturbation approximation for the collision-induced dipole of He...H, *J. Chem. Phys.* **84**, 3954-62 (1986).

17. K. L. C. Hunt and J. E. Bohr, Field-induced fluctuation correlations and the effects of van der Waals interactions on molecular polarizabilities, *J. Chem. Phys.* **84**, 6141-50 (1986).
18. J. E. Bohr and K. L. C. Hunt, Dipoles induced by van der Waals interactions during collisions of atoms with heteroatoms or with centrosymmetric linear molecules, *J. Chem. Phys.* **86**, 5441-48 (1987).
19. J. E. Bohr and K. L. C. Hunt, Dipoles induced by long-range interactions between centro-symmetric linear molecules: Theory and numerical results for  $H_2 \dots H_2$ ,  $H_2 \dots N_2$ , and  $N_2 \dots N_2$ , *J. Chem. Phys.* **87**, 3821-32 (1987).
20. K. L. C. Hunt, P. M. Hunt, and J. Ross, Dissipation in steady states of chemical systems and deviations from minimum entropy production, *Physica A* **147**, 48-60 (1987).
21. John Ross, Katharine L. C. Hunt, and Paul M. Hunt, Thermodynamics far from equilibrium: Reactions with multiple stationary states, *J. Chem. Phys.* **88**, 2719-29 (1988).
22. K. L. C. Hunt, Y. Q. Liang, and S. Sethuraman, Transient, collision-induced changes in polarizability for atoms interacting with linear, centrosymmetric molecules at long range, *J. Chem. Phys.* **89**, 7126-7138 (1988).
23. K. L. C. Hunt, P. M. Hunt, and John Ross, Deviations from minimum entropy production at steady states of reacting chemical systems arbitrarily close to equilibrium, *Physica A* **154**, 207-11 (1988).
24. Katharine L. C. Hunt, Paul M. Hunt, and John Ross, On Liapunov functions for single-variable reacting systems displaced from equilibrium, *J. Chem. Phys.* **90**, 880-87 (1989).
25. K. L. C. Hunt, Relationships between electric field shielding tensors and infrared or Raman intensities: An explanation based on nonlocal polarizability densities, *J. Chem. Phys.* **90**, 4909-15 (1989).
26. K. L. C. Hunt, Y. Q. Liang, R. Nimalakirithi, and R. A. Harris, Changes in electronic polarizability densities due to shifts in nuclear positions, and a new interpretation for integrated intensities of vibrational Raman bands, *J. Chem. Phys.* **91**, 5251-54 (1989).
27. K. L. C. Hunt, Dispersion dipoles and dispersion forces: Proof of Feynman's "conjecture" and generalization to interacting molecules of arbitrary symmetry, *J. Chem. Phys.* **92**, 1180-87 (1990).
28. P. M. Hunt, K. L. C. Hunt, and J. Ross, Thermodynamic and stochastic theory for nonequilibrium systems with more than one reactive intermediate: Non-autocatalytic and equilibrating systems, *J. Chem. Phys.* **92**, 2572-81 (1990).
29. K. L. C. Hunt, P. M. Hunt, and J. Ross, Nonlinear dynamics and thermodynamics of chemical reactions far from equilibrium, *Ann. Rev. Phys. Chem.* **41**, 409-39 (1990).
30. Katharine L. C. Hunt and Robert A. Harris, Vibrational circular dichroism and electric-field shielding tensors: A new physical interpretation based on nonlocal susceptibility densities, *J. Chem. Phys.* **94**, 6995-7002 (1991).
31. K. L. C. Hunt and Y. Q. Liang, Forces on nuclei in interacting molecules: New analytical results obtained with nonlocal polarizability densities, *J. Chem. Phys.* **95**, 2549-59 (1991).
32. John Ross, Katharine L. C. Hunt, and Paul M. Hunt, Thermodynamic and stochastic theory for non-equilibrium systems with multiple reactive intermediates: The concept and role of excess work, *J. Chem. Phys.* **96**, 618-29 (1992).
33. Qiang Zheng, John Ross, Katharine L. C. Hunt, and Paul M. Hunt, Stationary solutions of the master equation for single and multi-intermediate autocatalytic chemical systems, *J. Chem. Phys.* **96**, 630-40 (1992).
34. Katharine L. C. Hunt, J. Kottalam, Michael D. Hatlee, and John Ross, Multiple steady states in coupled flow tank reactors, *J. Chem. Phys.* **96**, 7019-33 (1992).

35. K. L. C. Hunt, P. M. Hunt, B. Peng, X. Chu, and J. Ross, The role of excess work in non-equilibrium thermodynamic systems, in *Spatio-Temporal Organization in Nonequilibrium Systems*, edited by S. C. Müller and T. Plesser (Projekt Verlag, Dortmund, 1992), 102-4.
36. R. Nimalakirithi and K. L. C. Hunt, Nonlocal polarizability density of a model system: A homogeneous electron gas at  $T = 0$ , *J. Chem. Phys.* **98**, 3066-75 (1993).
37. Ying Q. Liang and K. L. C. Hunt, Intramolecular screening of intermolecular forces, *J. Chem. Phys.* **98**, 4626-35 (1993).
38. X. L. Chu, J. Ross, P. M. Hunt, and K. L. C. Hunt, Thermodynamic and stochastic theory of reaction-diffusion systems with multiple stationary states, *J. Chem. Phys.* **99**, 3444-54 (1993).
39. P.-H. Liu and K. L. C. Hunt, Force balance and force relay in molecular interactions: An analysis based on nonlocal polarizability densities, *J. Chem. Phys.* **100**, 2800-07 (1994).
40. P. W. Fowler, K. L. C. Hunt, H. M. Kelly, and A. J. Sadlej, Multipole polarizabilities of the helium atom and collision-induced polarizabilities of pairs containing He or H atoms, *J. Chem. Phys.* **100**, 2932-35 (1994).
41. X. Li and K. L. C. Hunt, Transient changes in polarizability for centrosymmetric linear molecules interacting at long range: Theory and numerical results for  $H_2 \dots H_2$ ,  $H_2 \dots N_2$ , and  $N_2 \dots N_2$ , *J. Chem. Phys.* **100**, 7875-89 (1994).
42. X. Li and K. L. C. Hunt, Transient, collision-induced dipoles in pairs of centrosymmetric, linear molecules at long range: Results from spherical-tensor analysis, *J. Chem. Phys.* **100**, 9276-78 (1994).
43. K. L. C. Hunt and X. Li, Collision-induced dipoles and polarizabilities for S state atoms or diatomic molecules, *Collision- and Interaction-Induced Spectroscopy*, edited by G. C. Tabisz and M. N. Neuman, NATO ASI Ser. C **452** (Kluwer, Dordrecht, 1995), 61-76.
44. Bo Peng, Katharine L. C. Hunt, Paul M. Hunt, Alberto Suárez, and John Ross, Thermodynamic and stochastic theory of nonequilibrium systems: Fluctuation probabilities and excess work, *J. Chem. Phys.* **102**, 4548-62 (1995).
45. Alberto Suárez, John Ross, Bo Peng, Katharine L. C. Hunt, and Paul M. Hunt, Thermodynamic and stochastic theory of nonequilibrium systems: A Lagrangian approach to fluctuations and relation to excess work, *J. Chem. Phys.* **102**, 4563-73 (1995).
46. K. L. C. Hunt, Vibrational force constants and anharmonicities: Relation to polarizability and hyperpolarizability densities, *J. Chem. Phys.* **103**, 3552-60 (1995).
47. E. L. Tisko, X. Li, and K. L. C. Hunt, Relation of vibrational hyper-Raman intensities to  $\gamma$  hyperpolarizability densities, *J. Chem. Phys.* **103**, 6873-79 (1995).
48. P.-H. Liu and K. L. C. Hunt, Molecular softness, hypersoftness, infrared absorption, and vibrational Raman scattering: New relations derived from nonlocal polarizability densities, *J. Chem. Phys.* **103**, 10597-604 (1995).
49. X. Li and K. L. C. Hunt, Non-additive, three-body dipoles and forces on nuclei: New interrelations and an electrostatic interpretation, *J. Chem. Phys.* **105**, 4076-93 (1996).
50. X. Li, K. L. C. Hunt, J. Pipin, and D. M. Bishop, Long-range, collision-induced hyperpolarizabilities of atoms or centrosymmetric linear molecules: Theory and numerical results for pairs containing H or He, *J. Chem. Phys.* **105**, 10954-68 (1996).
51. X. Li and K. L. C. Hunt, Nonadditive three-body dipoles of inert gas trimers and  $H_2 \dots H_2 \dots H_2$ : Long-range effects in far infrared absorption and triple vibrational transitions, *J. Chem. Phys.* **107**, 4133-53 (1997).

52. X. Li, M. H. Champagne, and K. L. C. Hunt, Long-range, collision-induced dipoles of  $T_d-D_{\infty h}$  molecule pairs: Theory and numerical results for  $CH_4$  or  $CF_4$  interacting with  $H_2$ ,  $N_2$ ,  $CO_2$ , or  $CS_2$ , *J. Chem. Phys.* **109**, 8416-25 (1998).
53. M. H. Champagne, X. Li, and K. L. C. Hunt, Nonadditive three-body polarizabilities of molecules interacting at long range: Theory and numerical results for the inert gases,  $H_2$ ,  $N_2$ ,  $CO_2$ , and  $CH_4$ , *J. Chem. Phys.* **112**, 1893-1906 (2000).
54. K. L. C. Hunt, The energy as a functional of the charge density and the charge-density susceptibility: A simple, exact, nonlocal expression for the electronic energy of a molecule, *J. Chem. Phys.* **116**, 5440-47 (2002).
55. John Ross, Katharine L. C. Hunt, Marcel O. Vlad, Determination of thermodynamic and stochastic potentials in non-equilibrium systems from macroscopic measurements, *J. Phys. Chem. A* **106**, 10951-60 (2002).
56. Olga Spirina Jenkins and Katharine L. C. Hunt, Nonlocal dielectric functions on the nanoscale: Electronic polarization and fluctuations, *J. Mol. Struct. THEOCHEM* (issue in honor of D. M. Bishop) **633**, 145-155 (2003).
57. Dorothy J. Gearhart, James F. Harrison, and Katharine L. C. Hunt, Molecular quadrupole moments of HCCH, FCCF, and ClCCl, *Int. J. Quantum Chem.* **95**, 697-705 (2003).
58. Olga Spirina Jenkins and Katharine L. C. Hunt, Nonlocal dielectric functions on the nanoscale: Screened forces from unscreened potentials, *J. Chem. Phys.* **119**, 8250-56 (2003).
59. Michael Buser, Lothar Frommhold, Magnus Gustafsson, Massimo Moraldi, Mark H. Champagne, and K. L. C. Hunt, Far-infrared absorption by collisionally interacting nitrogen and methane molecules, *J. Chem. Phys.* **121**, 2617-21 (2004).
60. L. Frommhold and K. L. C. Hunt, Collision-induced spectra: About frame distortion, the hydrogen  $5\mu m$  band, and first-principle calculations, in *Spectral Line Shapes*, edited by L. Dalimier (Frontier Group, Paris, 2005), 37-44.
61. Katharine L. C. Hunt, A nonlocal energy functional derived from the fluctuation-dissipation theorem, ACS Symposium Series **958**, Electron Correlation Methodology, edited by Angela K. Wilson and Kirk A. Peterson (Am. Chem. Soc., Washington, DC, 2007), 169-182.
62. Edmund L. Tisko and Katharine L. C. Hunt, Derivatives of the polarization propagator including orbital relaxation effects, *J. Chem. Phys.* **126**, 204105 (2007).
63. X. Li, C. Ahuja, J. F. Harrison, and K. L. C. Hunt, The collision-induced polarizability of a pair of hydrogen molecules, *J. Chem. Phys.* **126**, 214302 (2007).
64. Dorothy J. Gearhart, Katharine L. C. Hunt, and James F. Harrison, The geometry, vibrational frequencies, thermochemistry, quadrupole moments and electronic structure of  $C_2Na_2$ : Comparison with  $C_2Li_2$ ,  $C_2H_2$ ,  $C_2F_2$  and  $C_2Cl_2$ , *J. Mol. Struct. THEOCHEM* **858**, 31-38 (2008).
65. Magnus Gustafsson, Lothar Frommhold, Xiaoping Li, and K. L. C. Hunt, Roto-translational Raman spectra of pairs of hydrogen molecules from first principles, *J. Chem. Phys.* **130**, 164314 (2009).
66. A. Mandal and K. L. C. Hunt, A single molecule as a dielectric medium, *J. Chem. Phys.* **131**, 234303 (2009).
67. Xiaoping Li, Katharine L. C. Hunt, Fei Wang, Martin Abel, and Lothar Frommhold, Collision-induced infrared absorption by molecular hydrogen pairs at thousands of Kelvin, *Int. J. Spectroscopy* **2010**, 371201 (2010).
68. Lothar Frommhold, Martin Abel, Fei Wang, Magnus Gustafsson, Xiaoping Li, and Katharine L. C. Hunt, Infrared atmospheric emission and absorption by simple molecular complexes, from first principles, *Mol. Phys.* **108**, 2265-2272 (2010).

69. Xiaoping Li, James F. Harrison, Magnus Gustafsson, Lothar Frommhold, and Katharine L. C. Hunt, The anisotropic polarizability of pairs of hydrogen molecules and the depolarized collision-induced roto-translational Raman light scattering spectra, invited article for a special issue in honor of Prof. Stanisław Kielich, *J. Comp. Methods Sci. Eng.* **10**, 367-399 (2010).
70. Lothar Frommhold, Martin Abel, Fei Wang, Xiaoping Li, and Katharine L. C. Hunt, Collision-induced absorption at temperatures of thousands of Kelvin, from first principles, for astrophysical applications, *20<sup>th</sup> International Conference on Spectral Line Shapes*, edited by John Lewis and Adriana Predoi-Cross, *AIP Conference Proceedings* **1290**, 219-230 (2010).
71. Martin Abel, Lothar Frommhold, Fei Wang, Magnus Gustafsson, Xiaoping Li, and Katharine L. C. Hunt, Collision-induced absorption by supermolecular complexes from a new potential energy and induced dipole surface, suited for calculations up to thousands of Kelvin, *20<sup>th</sup> International Conference on Spectral Line Shapes*, edited by John Lewis and Adriana Predoi-Cross, *AIP Conference Proceedings* **1290**, 251-257 (2010).
72. Martin Abel, Lothar Frommhold, Xiaoping Li, and Katharine L. C. Hunt, Collision-induced absorption by H<sub>2</sub> pairs: from hundreds to thousands of Kelvin, *J. Phys. Chem. A* **115**, 6805-6812 (2011).
73. Evangelos Miliordos and Katharine L. C. Hunt, First principles calculations of the electronic and geometrical structures of neutral [Sc, O, H] molecules and the monocations, ScOH<sup>0,+</sup> and HScO<sup>0,+</sup>, *J. Phys. Chem. A* **115**, 4436-4447 (2011).
74. Martin Abel, Lothar Frommhold, Xiaoping Li, and Katharine L. C. Hunt, Computation of collision-induced absorption by dense deuterium-helium gas mixtures, *J. Chem. Phys.* **134**, 076101 (2011).
75. Martin Abel, Lothar Frommhold, Xiaoping Li, and Katharine L. C. Hunt, Comparison of the calculated collision-induced absorption spectra by dense hydrogen-helium, deuterium-helium, and tritium-helium gas mixtures, *Journal of Atomic, Molecular, and Optical Physics* **2011**, 470530 (2011).
76. Evangelos Miliordos, James F. Harrison, and Katharine L. C. Hunt, *Ab initio* investigation of titanium hydroxide isomers and their cations, TiOH<sup>0,+</sup> and HTiO<sup>0,+</sup>, *J. Chem. Phys.* **135**, 144111 (2011).
77. Xiaoping Li, Anirban Mandal, Evangelos Miliordos, and Katharine L. C. Hunt, Interaction-induced dipoles of hydrogen molecules colliding with helium atoms: A new *ab initio* dipole surface for high-temperature applications, *J. Chem. Phys.* **136**, 044320 (2012).
78. Martin Abel, Lothar Frommhold, Xiaoping Li, and Katharine L. C. Hunt, Infrared absorption by collisional H<sub>2</sub>-He complexes at temperatures up to 9,000 K and frequencies from 0 to 20,000 cm<sup>-1</sup>, *J. Chem. Phys.* **136**, 044319 (2012).
79. Anirban Mandal and Katharine L. C. Hunt, Adiabatic and nonadiabatic contributions to the energy of a system subject to a time-dependent perturbation, *J. Chem. Phys.* **137**, 164109 (2012).
80. Xiaoping Li, James F. Harrison, Magnus Gustafsson, Fei Wang, Martin Abel, Lothar Frommhold, and Katharine L. C. Hunt, Collision-induced dipoles and polarizabilities of pairs of hydrogen molecules: *Ab initio* calculations and results from spherical tensor analysis, *AIP Conf. Proc.* **1504**, 100-135 (2012).
81. Evangelos Miliordos, James F. Harrison, and Katharine L. C. Hunt, Ground and excited states of vanadium hydroxide isomers and their cations, VOH<sup>0,+</sup>, and HVO<sup>0,+</sup>, *J. Chem. Phys.* **138**, 114305 (2013).
82. T. Karman, E. Miliordos, K. L. C. Hunt, G. C. Groenenboom, and A. van der Avoird, Quantum mechanical calculation of the collision-induced absorption spectra of N<sub>2</sub>-N<sub>2</sub> with anisotropic interaction, *J. Chem. Phys.* **142**, 084306 (2015).

83. Anirban Mandal and Katharine L. C. Hunt, Non-adiabatic current densities, transitions and power absorbed by a molecule in a time-dependent electromagnetic field, *J. Chem. Phys.* **143**, 034012 (2015).
84. Anirban Mandal and Katharine L. C. Hunt, Gauge-invariant expectation values of the energy of a molecule in an electromagnetic field, *J. Chem. Phys.* **144**, 044109 (2016).
85. Anirban Mandal and Katharine L. C. Hunt, Response to “Comment on ‘Gauge-invariant expectation value of the energy of a molecule in an electromagnetic field,’” *J. Chem. Phys.* **145**, 147103 (2016).
86. Anirban Mandal and Katharine L. C. Hunt, Quantum transition probabilities during a perturbing pulse: Differences between the nonadiabatic results and Fermi’s golden rule forms, *J. Chem. Phys.* **148**, 194107 (2018).
87. Anirban Mandal and Katharine L. C. Hunt, Nonadiabatic transition probabilities in a time-dependent Gaussian pulse or plateau pulse: Toward experimental tests of the differences from Dirac’s transition probabilities, *J. Chem. Phys.* **149**, 204110 (2018); *Journal of Chemical Physics* Editor’s Pick.
88. Evangelos Miliordos and Katharine L. C. Hunt, Dependence of the multipole moments, static polarizabilities, and static hyperpolarizabilities of the hydrogen molecule on the H-H separation in the ground singlet state, *J. Chem. Phys.* **149**, 234103 (2018).
89. Hua-Kuang Lee, Xiaoping Li, Evangelos Miliordos, and Katharine L. C. Hunt, The interaction-induced dipole of H<sub>2</sub>-H: New *ab initio* results and spherical tensor analysis, *J. Chem. Phys.* **150**, 204307 (2019); *Journal of Chemical Physics* Featured Article, AIP Scilight, and Editor’s Choice.
90. Anirban Mandal and Katharine L. C. Hunt, Variance of the energy of a quantum system in a time-dependent perturbation: Determination by nonadiabatic transition probabilities, *J. Chem. Phys.* **152**, 104110 (2020).
91. Anirban Mandal and Katharine L. C. Hunt, Quantum transition probabilities due to overlapping electromagnetic pulses: Persistent differences between Dirac’s form and nonadiabatic perturbation theory, *J. Chem. Phys.*, accepted for publication, 11/29/2020.
92. David Z. Wang, Aidan Q. Gauthier, Ashley E. Siegmund, and Katharine L. C. Hunt, Bell inequalities for entangled qubits: Quantitative tests of quantum character and nonlocality on quantum computers, submitted to *Phys Chem Chem Phys*, 10/16/2020.

#### Supervised Publications by Ph.D. Students

1. J. Juanós i Timoneda, Alternative derivation of perturbation expansions in the projection operator formalism, *Int. J. Quantum Chem.* **30**, 421-31 (1986).
2. Y. Q. Liang, H. Zhang, and Y. X. Dardenne, Momentum distributions for a particle in a box, *J. Chem. Ed.* **72**, 148 (1995).

#### Book Reviews

1. Katharine L. C. Hunt, *Dynamics of Synergetic Systems*, edited by H. Haken, *J. Am. Chem. Soc.* **102**, 7622 (1980).
2. Katharine L. C. Hunt, *Molecular Light Scattering and Optical Activity*, by L. D. Barron, *J. Am. Chem. Soc.* **105**, 7475-76 (1983).

## Conference Presentations

1. Katharine L. C. Hunt, Barbara A. Zilles, and James E. Bohr, Effects of van der Waals interactions on the polarizability of pairs of atoms, oscillators, and dipolar rotors, Midwest Theoretical Chemistry Conference, University of Chicago, 5/7/81-5/8/81.
2. Katharine L. C. Hunt and Barbara A. Zilles, Short-range correlation effects on pair polarizabilities, International Symposium on New Directions for the Molecular Theory of Gases and Liquids, University of Wisconsin, Madison, 6/18/81-6/20/81.
3. Katharine L. C. Hunt and John Ross, Path integral solutions of stochastic equations for nonlinear irreversible processes, American Conference on Theoretical Chemistry, University of Colorado, Boulder, 6/21/81-6/26/81.
4. Katharine L. C. Hunt, Nonlocal polarizability densities in the theory of collision-induced properties and van der Waals interactions at short range, Midwest Theoretical Chemistry Conference, Michigan State University, 4/30/82-5/1/82.
5. J. Kottalam and K. L. C. Hunt, Hysteresis in transitions between multiple nonequilibrium steady states, Midwest Theoretical Chemistry Conference, Michigan State University, 4/30/82-5/1/82.
6. Katharine L. C. Hunt, Nonlocal polarizability densities in the theory of collision-induced electrical properties of molecules, QELSS-I (First Conference on Quasi-Elastic Light Scattering Spectra and their Interpretations), University of Michigan, Ann Arbor, 6/23/82-6/25/82.
7. Katharine L. C. Hunt, Nonlocal polarizability densities: Applications to van der Waals interactions and to collision-induced properties, Gordon Research Conference on Atomic and Molecular Interactions, Brewster Academy, Wolfeboro, New Hampshire, 7/25/82-7/30/82.
8. Paul M. Hunt, Katharine L. C. Hunt, and John Ross, Applications of semiclassical methods in nonequilibrium thermodynamics, SERC Collaborative Computing Project (CCP6), Conference on Classical and Semiclassical Molecular Collisions and Dynamics, Warwick University, England, 4/21/83-4/22/83.
9. Katharine L. C. Hunt, A nonlocal polarizability density model for collision-induced properties, Midwest Theoretical Chemistry Conference, Northwestern University, 5/20/83-5/21/83.
10. J. Kottalam and K. L. C. Hunt, Transitions between multiple nonequilibrium steady states in the Schlögl model: Stochastic simulations and eigenvector analysis, Midwest Theoretical Chemistry Conference, Northwestern University, 5/20/83-5/21/83.
11. Paul M. Hunt, Katharine L. C. Hunt, and John Ross, Applications of semiclassical methods in nonequilibrium thermodynamics, Midwest Theoretical Chemistry Conference, Northwestern University, 5/20/83-5/21/83.
12. J. Kottalam and K. L. C. Hunt, Numerical studies of fluctuations and hysteresis in the homogeneous Schlögl model, Workshop on Fluctuations and Sensitivity in Nonequilibrium Systems, University of Texas at Austin, 3/12/84-3/16/84.
13. Katharine L. C. Hunt, J. Juanós i Timoneda, and James E. Bohr, Approximations for collision-induced dipoles and polarizabilities, American Conference on Theoretical Chemistry, Jackson Lake, Wyoming, 6/15/84-6/20/84.
14. Paul M. Hunt, Katharine L. C. Hunt, and J. Kottalam, Fluctuations and transitions in nonequilibrium systems with multiple steady states: Path integral techniques and master equation analysis, American Conference on Theoretical Chemistry, Jackson Lake, Wyoming, 6/15/84-6/20/84.
15. J. Ross and K. L. C. Hunt, Experiments and theory related to multiple steady states, Gordon Research Conference on Oscillations and Dynamic Instabilities in Chemical Systems, Plymouth, New Hampshire, 7/22/85-7/26/85.
16. K. L. C. Hunt, Effects of short-range interactions on molecular dipole moments and polarizabilities, Gordon Research Conference on Physics and Chemistry of Liquids, Holderness, New Hampshire, 8/19/85-8/23/85.



17. K. L. C. Hunt, Collision-induced changes in molecular dipoles and polarizabilities, Gordon Research Conference on Atomic and Molecular Interactions, Plymouth, New Hampshire, 7/28/86-8/1/86.
18. K. L. C. Hunt and J. E. Bohr, Collision-induced polarizabilities: The effects of van der Waals interactions, Tenth International Conference on Raman Spectroscopy, Eugene, Oregon, 8/31/86-9/ 5/86.
19. J. Juanós i Timoneda and K. L. C. Hunt, Interaction-induced dipole moment of  $H_3$  in the lowest quartet state, West Coast Theoretical Chemistry Conference, University of California, Berkeley, 6/ 10/87-6/12/87.
20. J. E. Bohr, J. Juanós i Timoneda, and K. L. C. Hunt, Transient, collision-induced changes in molecular dipoles and polarizabilities, American Conference on Theoretical Chemistry, Gull Lake, Minnesota, 7/27/87-7/31/87.
21. Y. Q. Liang and K. L. C. Hunt, Collision-induced changes in polarizability for atoms interacting with  $D_{2h}$  molecules at long range, Midwest Theoretical Chemistry Conference, Argonne National Laboratory, 5/13/88-5/14/88.
22. Katharine L. C. Hunt, Paul M. Hunt, and John Ross, Liapunov functions for reacting systems, Gordon Research Conference on Oscillations and Dynamic Instabilities in Chemical Systems, Plymouth, New Hampshire, 7/18/88-7/22/88.
23. K. L. C. Hunt, and Y. Q. Liang, Collision-induced changes in polarizability and Raman scattering by atom-diatom pairs, Eleventh International Conference on Raman Spectroscopy, London, England, 9/5/88-9/9/88.
24. Katharine L. C. Hunt, Infrared and vibrational Raman band intensities: A new physical interpretation based on nonlocal polarizability densities, Midwest Theoretical Chemistry Conference, University of Wisconsin, Madison, 5/17/90-5/19/90.
25. Paul M. Hunt, Katharine L. C. Hunt, and John Ross, Stochastic and thermodynamic theory for nonequilibrium systems with more than one reactive intermediate: Non-autocatalytic or equilibrating systems, Midwest Theoretical Chemistry Conference, University of Wisconsin, Madison, 5/17/90-5/19/90.
26. Ying Q. Liang, Srinivasan Sethuraman, and Katharine L. C. Hunt, Transient, collision-induced changes in polarizability for atoms interacting with linear, centrosymmetric molecules at long range, Midwest Theoretical Chemistry Conference, University of Wisconsin, Madison, 5/17/90-5/19/90.
27. R. Nimalakirithi, Ying Q. Liang, Katharine L. C. Hunt, and Robert A. Harris, Changes in electronic polarizability densities due to shifts in nuclear positions, Midwest Theoretical Chemistry Conference, University of Wisconsin, Madison, 5/17/90-5/19/90.
28. Ying Q. Liang, Srinivasan Sethuraman, and Katharine L. C. Hunt, Collision-induced changes in polarizability and Raman scattering by atom-diatom pairs, 10th International Conference on Spectral Line Shapes, University of Texas at Austin, 6/24/90-6/29/90.
29. Katharine L. C. Hunt, Infrared and vibrational Raman band intensities: A new physical interpretation based on nonlocal polarizability densities, 10th International Conference on Spectral Line Shapes, University of Texas at Austin, 6/24/90-6/29/90.
30. J. Ross, K. L. C. Hunt, and P. M. Hunt, Thermodynamics of nonlinear kinetic systems, American Conference on Theoretical Chemistry, San Diego, California, 7/29/90-8/3/90.
31. Katharine L. C. Hunt, Nonlocal polarizability densities: Applications in the theory of electric field shielding tensors, infrared and vibrational Raman band intensities, and dispersion forces, American Conference on Theoretical Chemistry, San Diego, California, 7/29/90-8/3/90.
32. Paul M. Hunt, Katharine L. C. Hunt, and John Ross, Stochastic and thermodynamic theory for nonequilibrium systems with multiple steady states, American Conference on Theoretical Chemistry, San Diego, California, 7/29/90-8/3/90.

33. Paul M. Hunt, Katharine L. C. Hunt, and John Ross, Stochastic and thermodynamic theory for nonequilibrium systems with multiple steady states: The role of the "excess" work required to reverse spontaneous changes in species concentrations, Midwest Theoretical Chemistry Conference, Northern Illinois University, 5/16/91-5/18/91.
34. Katharine L. C. Hunt and Robert A. Harris, Vibrational circular dichroism and electric-field shielding tensors: A new physical interpretation based on nonlocal susceptibility densities, Midwest Theoretical Chemistry Conference, Northern Illinois University, 5/16/91-5/18/91.
35. Ying Q. Liang and Katharine L. C. Hunt, Forces on nuclei in interacting molecules: New analytical results obtained with nonlocal polarizability densities, Midwest Theoretical Chemistry Conference, Northern Illinois University, 5/16/91-5/18/91.
36. Ying Q. Liang, Pao-Hua Liu, and Katharine L. C. Hunt, Intermolecular forces and intramolecular shielding: New results based on nonlocal polarizability densities, Midwest Theoretical Chemistry Conference, Michigan State University, 6/4/92-6/6/92.
37. Paul M. Hunt, Katharine L. C. Hunt, Bo Peng, and John Ross, On the concept and applications of "excess work" in nonequilibrium thermodynamic systems, Midwest Theoretical Chemistry Conference, Michigan State University, 6/4/92-6/6/92.
38. R. Nimalakirithi and Katharine L. C. Hunt, Functional form of the nonlocal polarizability density: Results for a homogeneous electron gas, taken as a model system, Midwest Theoretical Chemistry Conference, Michigan State University, 6/4/92-6/6/92.
39. X. Li and K. L. C. Hunt, Irreducible three-body forces, Gordon Conference on Atomic and Molecular Interactions, 7/4/94-7/8/94.
40. Edmund L. Tisko, Xiaoping Li, and Katharine L. C. Hunt, Changes in hyperpolarizabilities due to nuclear displacements, Midwest Theoretical Chemistry Conference, Northwestern University, 5/11/95-5/13/95.
41. Xiaoping Li and Katharine L. C. Hunt, Nonadditive three-body dipoles and three-body forces: An electrostatic interpretation, Midwest Theoretical Chemistry Conference, Northwestern University, 5/11/95-5/13/95.
42. Sandjaja Tjahajadiputra, Gary J. Blanchard, and Katharine L. C. Hunt, A test for correlations between vibrational Raman intensities and frequency-doubling tensors, Midwest Theoretical Chemistry Conference, Northwestern University, 5/11/95-5/13/95.
43. Pao-Hua Liu and Katharine L. C. Hunt, Force balance and force relay in molecular interactions, Midwest Theoretical Chemistry Conference, Northwestern University, 5/11/95-5/13/95.
44. E. L. Tisko, X. Li, and K. L. C. Hunt, Changes in nonlinear optical response tensors due to nuclear displacements, 210th American Chemical Society National Meeting, Chicago, 8/20/95-8/24/95.
45. X. Li and K. L. C. Hunt, Nonadditive three-body dipoles and forces: An electrostatic interpretation, 210th American Chemical Society National Meeting, Chicago, 8/20/95-8/24/95.
46. P.-H. Liu and K. L. C. Hunt, Molecular softness, infrared absorption, and vibrational Raman scattering: Relations derived from nonlocal polarizability densities, 210th American Chemical Society National Meeting, Chicago, 8/20/95-8/24/95.
47. P. M. Hunt, K. L. C. Hunt, B. Peng, and J. Ross, On the concept and applications of excess work in nonequilibrium thermodynamic systems, Ross Symposium, Stanford University, 4/12/97.
48. M. Yamato, K. L. C. Hunt, P. M. Hunt, and J. Ross, Electrochemical potentials in reacting nonequilibrium systems, Ross Symposium, Stanford University, 4/12/97.
49. X. Li, C. Ahuja, J. F. Harrison, and K. L. C. Hunt, *Ab initio* calculations of the charge-density susceptibility of the water molecule, 213th American Chemical Society National Meeting, San Francisco, California, 4/13/97-4/17/97.

50. Katharine L. C. Hunt, Nonlocal polarizability densities: Relation to infrared intensities, force constants, and van der Waals forces, Conference on Optical, Electric, and Magnetic Properties of Molecules, Cambridge, England, 7/10-97-7/13/97.
51. Xiaoping Li, Mark H. Champagne, and Katharine L. C. Hunt, Collision-induced dipole moments in  $T_d-D_{\infty h}$  molecule pairs at long range, American Conference on Theoretical Chemistry, Boulder, Colorado, 6/27/99-7/2/99.
52. Mark H. Champagne, Xiaoping Li, and Katharine L. C. Hunt, Nonadditive three-body polarizabilities of isotropic systems interacting at long range, American Conference on Theoretical Chemistry, Boulder, Colorado, 6/27/99-7/2/99.
53. Magnus Gustafsson, Lothar Frommhold, Xiaoping Li, James F. Harrison, and Katharine L. C. Hunt, Calculations of infrared and Raman spectral lineshapes in diatomic gases, 34th Meeting of the Division of Atomic, Molecular, and Optical Physics, American Physical Society, Boulder, CO, May 22, 2003.
54. Ruth C. Lafuente, Piotr Piecuch, and Katharine L. C. Hunt, Toward the development and implementation of computer programs for calculating the charge-density susceptibility, Midwest Theoretical Chemistry Conference, Iowa State University, June 12-14, 2003.
55. Dorothy J. Gearhart, James F. Harrison, and Katharine L. C. Hunt, Molecular quadrupole moments of HCCH, FCCF, and C1CC1, Midwest Theoretical Chemistry Conference, Iowa State University, June 12-14, 2003.
56. Anirban Mandal, Olga Spirina Jenkins, and Katharine L. C. Hunt, Nonlocal Dielectric Functions on the Nanoscale: Screening of Induction and Dispersion, International Workshop on Quantum Systems in Chemistry and Physics QSCP-XIII, Michigan State University, 7/11/2008.
57. Lothar Frommhold, Martin Abel, Fei Wang, K. L. C. Hunt, and Xiaoping Li, Collision-induced absorption at temperatures up to thousands of Kelvin from first principles, for astrophysical applications, invited talk by L. Frommhold at 20<sup>th</sup> International Conference on Spectral Line Shapes, St. John's, Newfoundland, Canada, 6/6/2010-6/11/2010.
58. Martin Abel, Lothar Frommhold, Xiaoping Li, and Katharine L. C. Hunt, Collision-induced infrared absorption by collisional complexes in dense hydrogen-helium gas mixtures at thousands of Kelvin, American Physical Society annual meeting, Division of Atomic, Molecular, and Optical Physics, Atlanta, GA, 6/16/2011.
59. Martin Abel, Lothar Frommhold, Xiaoping Li, and Katharine L. C. Hunt, Collision-induced infrared absorption by collisional complexes in dense hydrogen-helium gas mixtures at thousands of Kelvin, International Symposium on Molecular Spectroscopy, 66<sup>th</sup> meeting, Ohio State University, Columbus, OH, 6/24/2011.
60. Martin Abel, Lothar Frommhold, Xiaoping Li, and Katharine L. C. Hunt, Computation of collision-induced absorption by dense hydrogen-helium gas mixtures up to thousands of Kelvin, for astrophysical applications, Joint Fall 2011 Meeting of the Texas Sections of the APS, AAPT and Zone 13 of SPS, Texas A&M University, College Station, TX, 10/8/2011.
61. Martin Abel, Lothar Frommhold, Xiaoping Li, and Katharine L. C. Hunt, Computation of collision-induced absorption by dense hydrogen-helium gas mixtures up to thousands of Kelvin, for astrophysical applications, American Physical Society March Meeting, Boston, MA, 3/2/2012.
62. Evangelos Miliordos, James F. Harrison, and Katharine L. C. Hunt, *Ab initio* investigation of the MO and [M, O, H] systems, M = Sc, Ti, V, Midwest Theoretical Chemistry Conference, University of Wisconsin, Madison, 6/7/2012.
63. Xiaoping Li, Anirban Mandal, Evangelos Miliordos, and Katharine L. C. Hunt, Collision-induced absorption by hydrogen-hydrogen and hydrogen-helium pairs at high temperatures, Midwest Theoretical Chemistry Conference, University of Wisconsin, Madison, 6/7/2012.
64. Anirban Mandal and Katharine L. C. Hunt, Nonlocal dielectric model for intermolecular interactions at second order, Midwest Theoretical Chemistry Conference, University of Wisconsin, Madison, 6/7/2012.

65. Janelle Bradley, Sasha Brookhouse, and Katharine L. C. Hunt, Highly accurate potential energy surface for a hydrogen molecule interacting with a helium atom, Midwest Theoretical Chemistry Conference, University of Wisconsin, Madison, 6/7/2012.
66. Anirban Mandal and Katharine L. C. Hunt, Adiabatic and nonadiabatic contributions to the energy of a system subject to a time-dependent perturbation: Complete separation and physical interpretation, Midwest Theoretical Chemistry Conference, University of Illinois, Urbana-Champaign, 5/29/2013-5/31/2013.
67. Anirban Mandal and Katharine L. C. Hunt, Induction and dispersion forces on the nuclei of interacting molecules, Midwest Theoretical Chemistry Conference, University of Illinois, Urbana-Champaign, 5/29/2013-5/31/2013.
68. Janelle A. Bradley, Sasha Brookhouse, and Katharine L. C. Hunt, Accurate potential energy surface for the He-H<sub>2</sub> interacting system, for high-temperature astrophysical applications, Midwest Theoretical Chemistry Conference, University of Illinois, Urbana-Champaign, 5/29/2013-5/31/2013.
69. Zhongqi Jin, Evangelos Miliordos, and Katharine L. C. Hunt, Collision-induced dipole of H<sub>2</sub> · · · H, Graduate Research Symposium, Wayne State University, 9/28/2013.
70. Anirban Mandal and Katharine L. C. Hunt, Complete separation of the adiabatic and nonadiabatic contributions to the average energy of a system in the presence of a time-dependent perturbation, Midwest Theoretical Chemistry Conference, Northwestern University, 6/15/2014-6/17/2014.
71. Janelle A. Bradley, Sasha Brookhouse, and Katharine L. C. Hunt, Comparison of CCSD(T) and CR-CC(2,3) calculations of the potential energy surface for He-H<sub>2</sub>, Midwest Theoretical Chemistry Conference, Northwestern University, 6/15/2014-6/17/2014.
72. Anirban Mandal and Katharine L. C. Hunt, Perturbative approach to the adiabatic and nonadiabatic geometric phases of a multi-level quantum system, American Conference on Theoretical Chemistry, Telluride Science Research Center, 7/20/2014-7/25/2014.
73. Anirban Mandal and Katharine L. C. Hunt, Dispersion forces on nuclei of molecules within a dielectric framework, American Conference on Theoretical Chemistry, Telluride Science Research Center, 7/20/2014-7/25/2014.
74. Anirban Mandal and Katharine L. C. Hunt, Non-adiabatic current densities, transitions, and power absorbed by a molecule in a time-dependent electromagnetic field (talk), Midwest Theoretical Chemistry Conference, University of Michigan, 6/26/2015-6/28/2015.
75. Janelle Bradley and Katharine L. C. Hunt, Accurate potential energy surface for the He-H<sub>2</sub> interacting system, for high-temperature astrophysical applications, Midwest Theoretical Chemistry Conference, University of Michigan, 6/26/2015-6/28/2015.
76. Janelle Bradley and Katharine L. C. Hunt, Highly accurate potential energy surface for the He-H<sub>2</sub> interacting system, Midwest Theoretical Chemistry Conference, University of Michigan, 6/26/2015-6/28/2015.
77. Sasha Brookhouse, Evangelos Miliordos, and Katharine L. C. Hunt, Collision-induced properties of molecular oxygen, Midwest Theoretical Chemistry Conference, University of Michigan, 6/26/2015-6/28/2015.
78. Anirban Mandal and Katharine L. C. Hunt, Gauge-invariant expectation values of the energy of a molecule in an electromagnetic field (talk), Anirban Mandal and Katharine L. C. Hunt, Midwest Theoretical Chemistry Conference, University of Pittsburgh, 6/9/2016-6/11/2016.
79. Sasha Brookhouse, Evangelos Miliordos, and Katharine L. C. Hunt, Multipole moments and static (hyper)polarizabilities for the O<sub>2</sub> molecule, for atmospheric applications, Midwest Theoretical Chemistry Conference, University of Pittsburgh, 6/9/2016-6/11/2016.

80. Transition probabilities in quantum systems: Revisiting Fermi's Golden Rule, Midwest Theoretical Chemistry Conference, Michigan State University, 6/1/2107-6/3/2017.
81. Janelle Bradley and Katharine L. C. Hunt, Accurate potential energy surface for the He-H<sub>2</sub> interacting system, for high-temperature astrophysical applications, Midwest Theoretical Chemistry Conference, Michigan State University, 6/1/2107-6/3/2017.
82. Janelle Bradley and Katharine L. C. Hunt, Highly accurate potential energy surface for the He-H<sub>2</sub> interacting system, Midwest Theoretical Chemistry Conference, Michigan State University, 6/1/2107-6/3/2017.
83. Sasha Brookhouse, Evangelos Miliordos, and Katharine L. C. Hunt, Interactions between O<sub>2</sub> molecules, for atmospheric applications, Midwest Theoretical Chemistry Conference, Michigan State University, 6/1/2107-6/3/2017.
84. Anirban Mandal and Katharine L. C. Hunt, Differences between nonadiabatic transition probabilities and Fermi's golden rule results for a quantum system in the presence of a perturbing pulse, Midwest Theoretical Chemistry Conference, University of Chicago, 6/21/2018-6/23/2018.
85. Hua-Kuang Lee, Xiaoping Li, and Katharine L. C. Hunt, Collision-induced absorption by H<sub>2</sub>-H, Midwest Theoretical Chemistry Conference, University of Chicago, 6/21/2018-6/23/2018.
86. Anirban Mandal and Katharine L. C. Hunt, Nonadiabatic transition probabilities vs. Dirac's transition probabilities: Toward possible experimental tests for a quantum system in the presence of a plateau pulse (talk), Midwest Theoretical Chemistry Conference, Notre Dame, 6/6/2019-6/8/2019.
87. Hua-Kuang Lee, Xiaoping Li, Evangelos Miliordos, and Katharine L. C. Hunt, The interaction-induced dipole of H<sub>2</sub>-H, Midwest Theoretical Chemistry Conference, Notre Dame, 6/6/2019-6/8/2019.
88. Hua-Kuang Lee, Xiaoping Li, Evangelos Miliordos, and Katharine L. C. Hunt, Interaction-induced dipole of a hydrogen molecule colliding with a hydrogen atom, National Meeting of the American Chemical Society, 8/25/2019-8/29/2019.

### **Invited Lectures**

1. Path integrals and irreversible thermodynamics, Department of Chemistry, University of Michigan, 9/25/80.
2. Effects of short-range interactions on molecular properties, Department of Chemistry, Ball State University, 4/3/81.

3. Path integrals and nonlinear irreversible thermodynamics, Department of Chemistry, Yale University, 11/17/81.
4. Path integrals and nonlinear irreversible thermodynamics, Fluid Mechanics Division, Schlumberger-Doll Research, 2/2/82.
5. Collision-induced light scattering, Department of Chemistry, Wayne State University, 3/10/82.
6. Nonlocal polarizability densities and collision-induced spectroscopic processes, Department of Physics, University of Texas, Austin, 10/15/82.
7. Nonlocal polarizability densities and collision-induced spectroscopic processes, Department of Physics, University of Guelph, Ontario, 11/9/82.
8. Nonlocal polarizability densities and collision-induced properties, Department of Chemistry, University of Illinois at Chicago, 5/24/83.
9. Path integral solutions of stochastic differential equations describing nonequilibrium chemical systems, Conference on Path Integrals from meV to MeV, State University of New York at Albany, 8/1/83-8/5/83.
10. *Ab initio* and approximate calculations of collision-induced polarizabilities, NATO Advanced Research Workshop on Phenomena Induced by Intermolecular Interactions, Bonas, France, 9/5/83-9/9/83.
11. Collision-induced spectroscopic processes, Department of Physics, Université du Québec à Trois Rivières, Québec, 9/14/84.
12. Collision-induced spectroscopic processes and the effects of short-range interactions on molecular properties, Department of Chemistry, University of California, Berkeley, 3/26/85.
13. On the statistical mechanics of nonlinear irreversible processes, Theory seminar, Department of Chemistry, Stanford University, 3/29/85.
14. Collision-induced spectroscopic processes and the effects of short-range interactions on molecular properties, Department of Chemistry, University of Michigan, 4/18/85.
15. Path integral methods in nonequilibrium chemical thermodynamics, Conference on Path Integrals from meV to MeV, Bielefeld, West Germany, 8/5/85-8/9/85.
16. Effects of short-range interactions on molecular properties, with applications in collision-induced spectroscopy, Department of Chemistry, Indiana University, 4/3/86.
17. Nonequilibrium systems with multiple steady states: Path integral techniques and stochastic simulations, Institute for Nonlinear Dynamics, University of California, Davis, 5/29/86.
18. Effects of intermolecular interactions on dipole moments and polarizabilities, Theory seminar, Department of Chemistry, University of Minnesota, 10/7/86.
19. Collision-induced spectroscopic processes, Department of Chemistry, Oakland University, 10/21/87.
20. Light scattering, infrared absorption, and collision-induced properties, Department of Chemistry, University of Notre Dame, 11/5/87.
21. Molecular interaction effects and collision-induced spectra, Department of Chemistry, Indiana University-Purdue University at Indianapolis, 11/18/87.

22. Thermodynamic analysis of reacting systems displaced from equilibrium (with Paul M. Hunt), brief talk at the Gordon Research Conference on Oscillations and Dynamic Instabilities in Chemical Systems, Plymouth, New Hampshire, 7/22/88.
23. A unified view of electric-field shielding tensors, infrared intensities, and Raman intensities, Department of Chemistry, Wayne State University, 10/17/90.
24. Nonlocal polarizability densities: Applications in the theory of IR absorption, Raman scattering, and intermolecular interactions, American Chemical Society Joint Central-Great Lakes Regional Meeting, Indianapolis, 5/29/91.
25. Thermodynamic and stochastic theory of multiple steady state systems, Gordon Research Conference on Oscillations and Dynamic Instabilities in Chemical Systems, Newport, Rhode Island, 7/3/91.
26. Dispersion dipoles and dispersion forces: Proof of Feynman's conjecture, Condensed Matter Physics Seminar, Michigan State University, 9/26/91.
27. Intermolecular forces: Proof of Feynman's conjecture and characterization of intramolecular shielding, 203rd American Chemical Society National Meeting, Symposium on Intermolecular Forces, San Francisco, 4/6/92.
28. The role of "excess work" in nonequilibrium thermodynamic systems, Conference on Spatio-Temporal Organization in Nonequilibrium Systems, sponsored by the Max Planck Institut für Ernährungsphysiologie, the Initiativkreis Ruhrgebiet, and the European Community, Herdecke, Federal Republic of Germany, 6/22/92.
29. Collision-induced polarizabilities for diatomic molecule pairs, NATO Advanced Research Workshop on Induced Spectroscopy: Advances and Applications, Banff, Canada, 8/30/93.
30. Dispersion forces and dispersion dipoles: Proof of Feynman's conjecture, Department of Chemistry, University of California, Berkeley, 11/30/93.
31. Dispersion forces and dispersion dipoles: Proof of Feynman's conjecture, Department of Chemistry, Stanford University, 3/7/94.
32. Thermodynamic "excess work" and concentration fluctuations in reacting systems far from equilibrium, Gordon Research Conference on Modern Developments in Thermodynamics, 10/6/94.
33. Force constants, infrared intensities, and polarizabilities: Intramolecular origins, University of Michigan, Ann Arbor, 3/21/96.
34. Intermolecular forces: Connecting quantum and classical pictures, Michigan Technological University, 10/17/96.
35. Intermolecular forces: Connecting quantum and classical pictures, Eastern Michigan University, 10/28/96.
36. Stochastic and thermodynamic theory of nonequilibrium systems, Fifth North American Chemical Congress, Cancun, Mexico, 11/14/97.
37. Non-Nernstian electrochemical potentials and nonequilibrium thermodynamics, Gordon Conference on Modern Developments in Thermodynamics, Ventura, California, 3/11/01-3/16/01.
38. Nonlocal dielectric functions on the intramolecular scale, Midwest Theoretical Chemistry Conference, University of Minnesota, 10/4/01-10/6/01.
39. The energy as a functional of the charge density and the charge-density susceptibility: A simple, exact, nonlocal expression for the electronic energy of a molecule, 223rd American Chemical Society National Meeting, Symposium on Recent Advances in Electron Correlation Methodology, Orlando, Florida, 4/7/02-4/11/02.

40. Nonlocal susceptibilities and collision-induced properties, Department of Physics, University of Texas at Austin, 10/17/02.
41. Nanoscale dielectric functions: Nonlocal potential screening, 225th American Chemical Society National Meeting, Symposium on Integrating Diverse Computational Approaches to Complex Problem Solving, New Orleans, Louisiana, 3/23/03-3/27/03.
42. Collision-induced absorption and light scattering by hydrogen molecule pairs, International Conference on Quantum Systems in Chemistry and Physics, QSCP-XII, Royal Holloway College, University of London, Great Britain, 9/4/2007.
43. Collision-induced dipoles and polarizabilities of pairs of hydrogen molecules: *Ab initio* calculations and results from spherical tensor analysis, International Conference of Computational Approaches in Sciences and Engineering (ICCMSE), Rhodes, Greece, 9/29/09.
44. Collision-induced absorption by hydrogen molecule pairs and the spectra of cool white dwarf stars, International Conference on Quantum Systems in Chemistry and Physics, QSCP-XV, Cambridge, England, 8/31/2010-9/5/2010.
45. Collision-induced absorption by hydrogen molecule pairs and the spectra of cool white dwarf stars, Department of Chemistry, Wayne State University, 9/29/2010.
46. Interaction-induced dipoles of H<sub>2</sub>-He and the radiative profiles of cool white dwarf stars, International Conference of Computational Approaches in Sciences and Engineering (ICCMSE), Kos, Greece, 10/3/2010-10/8/2010.
47. Collision-induced infrared absorption and light scattering by interacting hydrogen molecules, Conference on Intermolecular Interactions: New Challenges for *ab initio* Theory, Telluride Scientific Research Center, Telluride, CO, 7/6/2015.
48. Advice on academic careers in science and engineering, Women in Science Conference, Notre Dame University, 9/30/2016-10/1/2016.
49. Thermodynamic and stochastic analysis of nonequilibrium systems, Symposium in honor of Professor John Ross, Stanford University, 5/19/2017.
50. Nonlocal dielectric theory of electrostatic, induction, and dispersion interactions, Telluride Scientific Research Conference on Intermolecular Interactions: New Challenges for *ab initio* Theory, Arenas de Cabrales, Spain, 7/8/2017-7/13/2017.
51. New *ab initio* results for collision-induced dipoles and polarizabilities and new analytical results for transition probabilities, Telluride Science Research Center workshop on Intermolecular Interactions: New Challenges for *ab initio* Theory, Telluride, CO, 3/18/2019-3/22/2019.
52. New *ab initio* results for interaction induced dipoles and susceptibilities and new analytical results for transition probabilities, 10th Congress of the International Society of Theoretical Chemical Physics (ISTCP), Tromsø, Norway, Scientific track on Molecular Properties and Interactions, 7/11/2019-7/17/2019.
53. Symposium in honor of Dr. Evelyn Goldfield on her retirement from the National Science Foundation, 9/16/2020  
*Upcoming invited talks:*  
American Conference on Theoretical Chemistry, Squaw Valley, CA, planned for Summer 2020, rescheduled to summer 2021.



25th International Workshop on Quantum Systems in Chemistry, Physics and Biology, Toruń, Poland, originally scheduled for 6/28/2020-7/3/2020, rescheduled to Summer 2021.

6<sup>th</sup> Conference on Nuclei and Mesoscopic Physics, Facility for Rare Isotope Beams, Michigan State University, rescheduled to 3/8/21-3/12/21.

Telluride Science Research Center workshop on Intermolecular Interactions: New Challenges for *ab initio* Theory, Arenas de Cabrales, Spain, Summer 2021.

International Conference on Quantum Chemistry, scheduled for New Zealand, 2024.

### **Research Grants**

1. ACS-PRF Type G Grant, *Ab initio* and approximate calculations of collision-induced dipoles and polarizabilities, \$10,000, 2/1/80-8/31/82.

2. MSU AURI Grant, Transitions between steady states, hysteresis, and instabilities in chemical systems far from equilibrium, \$5,000, 1/1/80-6/30/80.
3. Cottrell Research Grant, Research Corporation, Computer simulation of dynamic hysteresis effects in transitions between nonequilibrium steady states of chemical systems, \$20,000, joint grant with Prof. Paul M. Hunt, 6/6/80-6/30/82.
4. ACS-PRF Type AC Grant, *Ab initio* and approximate calculations of collision-induced dipoles and polarizabilities, \$30,000, 9/1/82-8/31/87.
5. National Science Foundation, Theory of transient, collision-induced changes in molecular dipoles and polarizabilities, \$177,012, 1/1/88-12/31/90.
6. National Science Foundation, Theory of transient, collision-induced changes in molecular dipoles and polarizabilities, \$246,000, 1/15/91-12/31/93.
7. National Science Foundation, Supplemental award to support research experience for undergraduates, \$3,300, 5/14/91-6/30/92.
8. MSU AURI Grant, Intramolecular response to inhomogeneous magnetic fields, \$10,000, 7/1/91-6/30/92.
9. National Science Foundation, New directions in the molecular theory of electromagnetic response and in nonequilibrium thermodynamics, Career Advancement Award, \$34,600, 9/1/93-8/31/94.
10. National Science Foundation, Nonlocal electromagnetic response: Theory and applications, \$300,000, 3/1/94-8/31/97.
11. National Science Foundation, Nonlocal electromagnetic response: Theory and applications, \$73,000, 10/1/97-12/31/98.
12. National Science Foundation, Purchase of a High-Performance Parallel Computer (Departmental Equipment Proposal), PI: K. L. C. Hunt, co-PIs: G. T. Babcock, J. F. Harrison, J. E. Jackson, P. Piecuch, \$200,000, 6/1/99-5/31/02.
13. National Science Foundation, Single-molecule trapping and nanoscale dielectric response, \$321,000, 3/1/99-2/28/04.
14. National Science Foundation, Absorption of radiation by hot, dense mixtures of hydrogen and helium, \$161,676, 8/1/07-7/31/11.
15. National Science Foundation, Theory and simulation of dye-labeled protein molecules in optical fields, PI: Katharine L. C. Hunt, Co-PI: Robert I. Cukier, \$420,000, 8/15/13-7/31/17.
16. National Science Foundation, Nonadiabatic Transition Probabilities: Applications in Spectroscopy and Quantum Thermodynamics, \$280,000, 8/1/19-7/31/21.
17. Herbert H. and Grace A. Dow Foundation, A Proposal for the 2019-2021 Support of MSU St. Andrews and Related Campus Resources, PI: Paul M. Hunt, Co-PIs: Katharine C. Hunt and Loraine J. Hudson, \$1,100,000, 5/1/19 – 4/30/21.
18. Rollin M. Gerstaecker Foundation and Charles J. Strosacker Foundation, A Proposal to the Rollin M. Gerstaecker Foundation and the Charles J. Strosacker Foundation for the 2020-2021 Support of MSU St. Andrews, PI: Paul M. Hunt, Co-PIs: Katharine C. Hunt and Loraine J. Hudson, \$525,000, 1/1/20-12/31/21.

***Also listed as Senior Personnel on the following pending proposals:***

1. National Science Foundation, NRT-QL: The Quantum Leap: Leading the Next Quantum Revolution, \$2,998,449, 8/16/20-8/15/25.

2. Department of Energy (DOE), Quantum Strategic Innovation and Development (QSID) Center, \$125,000,000 (a multi-institutional proposal), 10/1/20-9/30/25.

**Contribution to University-wide Proposal**

1. General Electric Foundation, Science and Engineering Faculty for the Future, Co-author (with Profs. Howard Anderson, Nicholas Altiero, and Michael Harrison) of Michigan State University proposal, \$330,000, 9/1/91-12/30/94.

**Proposal on behalf of Biomolecular Researchers at Michigan State University**

1. Center for Synthesis and Characterization of Biomolecules, MSU Foundation, \$1,500,000, 7/01/99-6/30/02.

**Research Group**

**Visiting Faculty**

Dr. Sean A. C. McDowell, FRS, Professor of Theoretical Chemistry, Department of Biological and Chemical Sciences, University of the West Indies, Cave Hill Campus, Barbados, Summers 2000, 2001, and 2002

#### **Postdoctoral Associates: Career Total, 9**

- Dr. Barbara Zilles (Ph.D., University of Florida, Gainesville, 1980; research advisor, Prof. Willis B. Person) MSU Affirmative Action Postdoctoral Fellow, 1980-81; MSU Research Associate, 1981-82; currently Applications Development and Support Staff, Health Care Information Systems, University of Iowa
- Dr. Xiaolin Chu (Ph.D., UNED, Spain, 1988; research advisor, Prof. M. Velarde), MSU Research Associate, 1990-91, joint postdoctoral associate with Prof. John Ross, Stanford University
- Dr. Bo Peng (Ph.D., University of West Virginia, 1991; research advisor, Prof. Kenneth Showalter), MSU Research Associate, 1992-95; financial analyst, Shearson-Lehmann until 2008; now independent portfolio manager
- Dr. Pao-Hua Liu (B.S., Fu Jen Catholic University, Taiwan, 1988) Ph.D., Michigan State University, 1995. Postdoctoral Research Associate, Michigan State University, 1995-96; Intel Corporation, Santa Clara, California
- Dr. Olga B. Spirina Jenkins (M. A., Chemistry, Novosibirsk State University, 1988) Ph.D., Michigan State University, 1995. Postdoctoral Research Associate, Michigan State University, 1995-2000, currently VP Marketing Database Manager, Wells Fargo Bank, San Francisco, California
- Dr. Xiaoping Li (B.S., Tsinghua University, P.R.C., 1987; M.S., Tsinghua University, 1989) Ph.D., Michigan State University, 1994. Postdoctoral Research Associate, Michigan State University, 1995-present (currently 25% appointment); Information Technologist III, Enterprise Business Systems Project, Office of the Vice President for Finance and Operations, MSU (75% appointment)
- Dr. Mark H. Champagne (B.S., Oakland University, 1991; M. A., Wayne State University, 1995) Ph.D., Michigan State University, 2000; Postdoctoral Research Associate, Michigan State University, 2001-02; Professor and Interim Associate Dean, Arts and Sciences, Macomb Community College
- Dr. Anirban Mandal (B.S., M.S., Indian Institute of Technology, Kanpur; Ph.D., Michigan State University, 2009) January 2010- January 2016, Senior Postdoctoral Research Associate, 2017-
- Dr. Evangelos Miliordos (Ph.D. National and Kapodistrian University of Athens, Greece, 2010), May 2010-2012; currently Assistant Professor of Chemistry, Auburn University

#### **Ph.D. Graduates: Career Total, 16**

- J. Kottalam (B.Sc., A. M. Jain College, University of Madras, 1975; M.Sc., Indian Institute of Technology, Madras, 1978) Ph.D., Michigan State University, 1984. Research Associate, University of California, San Diego, 1984-86; Research Associate, Scripps Clinic and Research Foundation, La Jolla, 1986-1989; Research Associate, Harvard University, 1989-1990; Accelrys, 1991-93; CRAY, 1994-96; Structural Bioinformatics, Inc. 1996-2003; Kuylian BioSoft Corp., 2003-2004; Pfizer Pharmaceuticals, 2007-2008; Reaction Design, 2008-present
- Jesús Juanós i Timoneda (M.Lic., University of Barcelona, 1981; Caixa de Barcelona Research Fellow, 1982-83; SOHIO Fellow, 1985-86) Ph.D., Michigan State University, 1986. Research Associate, University of California, Berkeley, 1986-1988; Research Associate, University of Utah, 1988-1990; Research Associate, University of Colorado, Boulder, 1990-1992; Attorney, Johnson & Johnson Pharmaceutical Research & Development, LLC
- James E. Bohr (B.S., Michigan State University, 1981; NSF Predoctoral Fellow, 1981-84; College of Natural Science Continuing Doctoral Fellow, 1985-86) Ph.D., Michigan State University, 1987. National Research Council Postdoctoral Associate, AFSC/AFRPL Program, Edwards Air Force Base, 1987-1989; Michigan Consortium for Enabling Technologies; Michigan Disability Rights Coalition
- Ying Q. Liang (B.S., Guangxi University, P.R.C., 1962; Faculty member on leave from Physics Department, Guangxi University), Ph. D., Michigan State University, 1992. Postdoctoral Research

Associate, Colorado State University, 1992-93; Manager, MDSM Data Analysis Services LLC (retired)

R. Nimalakirithi (B.Sc., University of Colombo, Sri Lanka, 1982) Ph.D., Michigan State University, 1993. Postdoctoral Research Associate, Texas A&M University, Research Scientist, Optimal Air Products, 1994-

Xiaoping Li (B.S., Tsinghua University, P.R.C., 1987; M.S., Tsinghua University, 1989) Ph.D., Michigan State University, 1994. Postdoctoral Research Associate, Michigan State University, 1995- present (currently 25% appointment); Information Technologist III, Enterprise Business Systems Project, Office of the Vice President for Finance and Operations, MSU (75% appointment).

Glenda Soriano (B.S., University of the Philippines, 1986; M.S., University of the Philippines, 1989; joint student with Profs. R. H. Schwendeman and P. M. Hunt), Ph.D., Michigan State University, 1995. Postdoctoral Research Associate, Purdue University, 1995; Research Scientist, Roche Diagnostics; Adjunct Lecturer, Indiana University/Purdue University; currently Postdoctoral Research Associate, Biological Sciences, Purdue University

Pao-Hua Liu (B.S., Fu Jen Catholic University, Taiwan, 1988), Ph.D., Michigan State University, 1995. Intel Corporation, Santa Clara, California.

Ed Tisko (B.S., Michigan Tech, 1988), Ph.D., Michigan State University, 1998, currently Assistant Professor of Chemistry, University of Nebraska, Omaha

Mark Champagne (B.S., Oakland University, 1991; M. A., Wayne State University, 1995), Ph.D., Michigan State University, 2000; Professor of Chemistry and Interim Associate Dean, Arts and Sciences, Macomb Community College

Ruth Lafuente Jacobsen (B.S., University of Rochester, 1999), Ph.D., Michigan State University, 2006; joint student with Prof. Piotr Piecuch; Lumsden-Valrance Lecturer, Michigan State University; Analyst, Center for Naval Analyses, 2007-2009; Visiting Senior Research Scientist, National Institute of Standards and Technology, 2011-

Dorothy Gearhart (B. S., University of Montevallo, Alabama, 1999), Ph.D. Michigan State University, 2007; joint student with Prof. James Harrison; Adjunct Instructor, Chemistry and Physics, Auburn University at Montgomery, Alabama.

Anirban Mandal (B.S., M.S., Indian Institute of Technology, Kanpur), Ph.D., Michigan State University, 2009; Postdoctoral Research Associate, Michigan State University, 2010-2016; Senior Postdoctoral Research Associate, Michigan State University, 2016-

Sasha Brookhouse North (B.S., Michigan State University), Ph.D., Michigan State University, 2016; Visiting Professor of Chemistry, Grand Valley State University; currently Postdoctoral Research Associate, group of Prof. Angela Wilson, MSU

Janelle Bradley (B.S., Chemistry and Mathematics, Michigan State University), transferred from the group of Prof. Piotr Piecuch, Spring 2011, Ph.D. Michigan State University, 2018, Scientific Staff Member at MSU St. Andrews Facility, Midland, MI

Jin Chi, Ph.D., Michigan State University, 2019 (jointly supervised by K. L. C. Hunt and R. I. Cukier), Pillar Biosciences

### **Current Ph.D. Students, 2**

Hua-Kuang Lee (B.S., University of Minnesota)

Nathan Jansen (B.S., Portland State University, Oregon)

### **Post-Baccalaureate Research Assistant**

Julianne Van Wagenen, B.A., Depaul University Honors College, 2006; Università degli Studi Roma Tre, Italy, Biology Department, 2006-08, Ph.D. Harvard University.

## **Undergraduate Research Assistants**

Kania Adams (B. S., Michigan State University, 2002)  
Sean Burns (B. S., University of Michigan, 1994), National Science Foundation Research Experience for Undergraduates, Summer 1992  
Rose Cory (B. S., Michigan State University, 1998), NSF REU Student, 1997  
LaShawn Ford (B.S., Michigan State University, 1993)  
Douglas Garrity (B.S., Michigan State University, 1981; Ph.D., Columbia University, 1986)  
Lisa Green (B.S., Michigan State University, 2005); NSF REU Student, 2004  
Stephen Jarboe (B.S., Transylvania College, 1997), NSF REU Student, 1996  
Kara Johnson (B.S., Marietta College, 1994), NSF REU Student, 1993  
Mark Kubinec (B.S., Michigan State University, 1987; Ph.D., Berkeley)  
C. Michael McCallum (B.S., Michigan State University, 1988; Ph.D., Berkeley)  
Manjula Samuel (B. S., Michigan State University, 1999), McNair/SROP Student, 1997  
Kristin Taylor (B. S., Michigan State University, 1999), NSF REU Student, 1997  
Mark D. Toatley (B.S., Eastern Michigan University, 1997), NSF REU Student, 1995  
Catherine Tloczynski (B.S., Alma College, 1993), General Electric Foundation Summer Research Student, 1992  
Jason Wengert (B.S., Michigan State University, 2006)  
Brian Wentzloff (B.S., Michigan State University, 2006)  
Garrett Marushia-Laurain (B.S., Michigan State University, 2008)  
Vatsal Bajpai (B.A., Kalamazoo College, 2010)  
Ryan Hendricks (B.S., Michigan State University, 2010)  
David Dombrowski (B.S., Michigan State University, 2103)  
Ray Szeto (B.S., Michigan State University, 2107)  
David King (B.S., Michigan State University, 2017)  
Sara Bollstetter (B.S., Michigan State University, 2018)  
John Buell (B.S. expected, Michigan State University, 2021)

## **High-School Student Researchers**

Benjamin Edwards, High School Honors Science Program at Michigan State University, participant from Half Hollow Hills High School, Dix Hills, New York, Summer 2015, Intel Science Talent Search Semifinalist  
Bogdan Manga, High School Honors Science Program at Michigan State University, participant from the International Academy, Bloomfield Hills, Michigan, Summer 2016, Intel Science Talent Search Semifinalist, Siemens Competition in Math, Science, and Engineering, Semifinalist.  
Aidan Gauthier, quantum computing, MSU St. Andrews Summer Internship Program, 2019 and 2020  
Ashley Siegmund, quantum computing, MSU St. Andrews Summer Internship Program, 2019 and 2020  
Guanghan (Henry) Ma, quantum computing, MSU St. Andrews Summer Internship Program, 2019  
David Wang, quantum computing, MSU St. Andrews Summer Internship Program, 2019 and 2020  
Julia Egbert, quantum computing, MSU St. Andrews Summer Internship Program, 2020  
Corbin Fleming-Dittenber, quantum computing, MSU St. Andrews Summer Internship Program, 2020  
Scott Gilbert, quantum computing, MSU St. Andrews Summer Internship Program, 2020  
Zbynek Hlavacek, quantum computing, MSU St. Andrews Summer Internship Program, 2020  
Matthew Loucks, quantum computing, MSU St. Andrews Summer Internship Program, 2020  
Garrett Mai, quantum computing, MSU St. Andrews Summer Internship Program, 2020  
Jessica Messing, quantum computing, MSU St. Andrews Summer Internship Program, 2020  
Andrew Scheffer, quantum computing, MSU St. Andrews Summer Internship Program, 2020

## **Teaching**

W'80      CEM 985      Nonequilibrium Statistical Mechanics

S'80	CEM 985	Equilibrium Statistical Mechanics
F'80	CEM 998	Physical Chemistry Seminar
W'81	CEM 987	Nonequilibrium Statistical Mechanics
	CEM 998	Physical Chemistry Seminar
S'81	CEM 985	Equilibrium Statistical Mechanics
	CEM 998	Physical Chemistry Seminar
W'82	CEM 985	Nonequilibrium Statistical Mechanics
S'82	CEM 985	Equilibrium Statistical Mechanics
W'83	CEM 991	Quantum Chemistry
S'83	CEM 991	Electric and Magnetic Properties of Molecules, Intermolecular Forces
F'83	CEM 181H	Honors Chemistry I - Principles
	CEM 184H	Honors Chemistry Laboratory I
	CEM 499	Seminar on Chemical Physics
W'84	CEM 182H	Honors Chemistry II - Principles
	CEM 185H	Honors Chemistry Laboratory II
	CEM 499	Seminar on Chemical Physics
F'84	CEM 181H	Honors Chemistry I - Principles
	CEM 184H	Honors Chemistry Laboratory I
W'85	CEM 182H	Honors Chemistry II - Principles
	CEM 185H	Honors Chemistry Laboratory II
<i>Academic Year 1985-86, Sabbatical at Stanford University</i>		
W'87	CEM 991	Quantum Chemistry
S'87	CEM 985	Equilibrium Statistical Mechanics
W'88	CEM 991	Quantum Chemistry
S'88	CEM 985	Equilibrium Statistical Mechanics
F'88	CEM 998	Physical Chemistry Seminar
W'89	CEM 991	Quantum Chemistry
	CEM 998	Physical Chemistry Seminar
S'89	CEM 991	Special Topics in Quantum Chemistry
	CEM 998	Physical Chemistry Seminar
W'90	CEM 185H	Honors Chemistry Laboratory II
	CEM 991	Quantum Chemistry
S'90	CEM 988	Special Topics in Physical Chemistry
W'91	CEM 362	Analytical/Physical Chemistry I
S'91	CEM 988	Special Topics in Physical Chemistry: Scattering Theory
W'92	CEM 991	Quantum Chemistry
S'92	CEM 985	Equilibrium Statistical Mechanics
	CEM 499	Seminar in Chemical Physics
S'93	CEM 992	Quantum Chemistry and Statistical Thermodynamics II
<i>Academic Year 1993-1994, Sabbatical at Stanford University</i>		
F'94	CEM 181H	Honors Chemistry I - Principles
F'95	CEM 181H	Honors Chemistry I - Principles
F'96	CEM 991	Quantum Chemistry and Statistical Thermodynamics I
F'97	CEM 991	Quantum Chemistry and Statistical Thermodynamics I
<i>Academic Years 1998-1999 through 2001-2002, Department Chairperson</i>		
S'03	CEM 992	Quantum Chemistry and Statistical Thermodynamics II
S'04	CEM 992	Quantum Chemistry and Statistical Thermodynamics II
S'05	CEM 384	Introductory Physical Chemistry II
	CEM 992	Quantum Chemistry and Statistical Thermodynamics II
S'06	CEM 384	Introductory Physical Chemistry II
S'07	CEM 384	Introductory Physical Chemistry II
S'08	CEM 384	Introductory Physical Chemistry II
S'09	CEM 499	Chemical Physics Seminar
	CEM 992	Quantum Chemistry and Statistical Thermodynamics II
S'10	CEM 499	Chemical Physics Seminar

	CEM 992	Quantum Chemistry and Statistical Thermodynamics II
S'11	CEM 499	Chemical Physics Seminar
	CEM 992	Quantum Chemistry and Statistical Thermodynamics II
S'12	CEM 499	Chemical Physics Seminar
	CEM 992	Quantum Chemistry and Statistical Thermodynamics II
S'13	CEM 499	Chemical Physics Seminar
	CEM 992	Quantum Chemistry and Statistical Thermodynamics II
S'14	CEM 186	Honors General Chemistry Laboratory
	CEM 499	Chemical Physics Seminar
S'14	CEM 992	Quantum Chemistry and Statistical Thermodynamics II
S'15	CEM 499	Chemical Physics Seminar
	CEM 992	Quantum Chemistry and Statistical Thermodynamics II
S'16	CEM 484	Molecular Thermodynamics
	CEM 499	Chemical Physics Seminar
S'17	CEM 484	Molecular Thermodynamics
	CEM 499	Chemical Physics Seminar
S'18	CEM 484	Molecular Thermodynamics
	CEM 499	Chemical Physics Seminar
US'18	CEM 987	Special Topics in Physical Chemistry: Applicable Mathematics
S'19	CEM 484	Molecular Thermodynamics
	CEM 499	Chemical Physics Seminar
US'19	CEM 987	Special Topics in Physical Chemistry: Applicable Mathematics
S'20	CEM 484	Molecular Thermodynamics
	CEM 499	Chemical Physics Seminar

### **Undergraduates Directed in Research Courses**

#### **CEM 186H**

David Rosenbaum, S'81  
Stanley Heckman, S'83  
Renée Szostek, S'87  
Guy Albertelli, S'93  
Daniel Hornbaker, S'93  
Lawrence Su, S'93  
William Schmitt, S'95  
Kristin Taylor, S'96  
Ferenc Nagy, S'96  
Elizabeth Pfaff, S'00  
David Dombrowski, S'10  
David King, S'14

#### **CEM 400H**

James Bohr, W'80, S'80  
Mark Finzel, W'80, S'80  
David Rosenbaum, F'81-F'82  
Steven Cuccaro, W'82-F'82  
Michael McCallum, F'87  
Rose Cory, S'97  
Sara Dushanka Jovanovski, S'20, F'20

#### **CEM 419**

Michael Richmann, W'84-S'85  
Michael McCallum, S'87



Jim Vivian, S'87, F'87  
Stephen Stahel, S'88  
Masanori Yamato, F'96

***Departmental and College Service***

Advisory Committee (7/1/80-6/30/82, 7/1/91-6/30/93, 7/1/96-6/30/98)  
Awards Committee (7/1/81-6/30/82, 7/1/94-6/30/95, 7/1/2019-6/30/2020)

Bylaws Committee (2002-03)  
Chair Search Committee (2010), Chair  
Chemical Physics Committee (3/23/81-6/30/82, 7/1/84-6/30/85, 10/20/87-6/30/88)  
Chair (1/4/82-6/30/82)  
Colloquium Committee (7/1/80-6/30/81)  
Educational Policies Committee (7/1/90-6/30/91, 7/1/94-6/30/95, 7/1/97-6/30/98)  
Chair (7/1/90-6/30/91)  
Faculty Search and Selection Committees  
Organic Chemistry (1980, 1991-92, 1994-95, 1996-97)  
Nuclear Chemistry (1981)  
Chemical Engineering (1981-82)  
Analytical, Inorganic, and Organic Chemistry (1982-83)  
Analytical and Inorganic Chemistry (1983-84)  
Physical Chemistry (1987-88, 1988-89, 1992-93, 1997-98)  
X-ray Crystallography (1994-95)  
Open Across Areas (2013-14)  
Open Across Areas (2014-15)  
Theoretical Chemistry (2015-16)  
Graduate Admissions Committee (7/1/82-6/30/84, 7/1/88-6/30/90, 7/1/2016-6/30/18, 7/1/19-6/30/21)  
Graduate Advising Committee (7/1/83-6/30/85, 7/1/89-6/30/91, 7/1/2017-6/30/19, 7/1/20- )  
Library Committee (7/1/90-6/30/92)  
Chair (7/1/91-6/30/92)  
Physical Chemistry Graduate Recruiting Coordinator (11/12/87-6/30/88)  
Quill Fellowship Interview Panel (1982-84, 1988, 1989)  
Reappointment and Promotions Committee (7/1/84-6/30/85, 7/1/86-6/30/88, 7/1/95-6/30/96, 7/1/2010-6/30/2010), Chair (7/1/95-6/30/96)  
Safety Committee (2002-03)  
College of Natural Science Scholarship Committee (7/1/2009-6/30/2011)  
College of Natural Science Reappointment and Promotions Committee (7/1/2010-6/30/2012)

***Service as Department Chairperson, Michigan State University, 1998-2002***

*Faculty Hiring, Set-Up, and Promotion*

4 faculty hires (Professors Jim McCusker, Greg Swain, Jetze Tepe, and Bill Wulff), 3 at a senior level  
5 faculty set-ups, with laboratory renovations (4 hires + Professor Aaron Odom)  
8 tenure decisions  
5 promotions to Full Professor

*Department Funding*

Research funding of the MSU Department of Chemistry rose significantly during term as Chairperson (1998-2002); data from earlier years are included to show a baseline level. The Department substantially increased both federally funded research grant expenditures and total expenditures for research in Chemistry with proposals submitted during the term as Chairperson, and more than doubled NIH funding in a one-year period. The Department rose to 32nd in the country in total expenditures for chemical research (up from a national ranking in the 50-55 range), and remained in the 30-40 range through 2007.

*Federal Research Grant Expenditures, MSU Chemistry:*

1994-95	\$3.714 M
1995-96	\$4.399 M
1996-97	\$4.378 M
1997-98	\$3.541 M
1998-99	\$3.790 M
1999-00	\$4.568 M
2000-01	\$7.857 M
2001-02	\$6.748 M
2002-03	\$6.297 M

*Total Grant Expenditures for Chemical Research, MSU Chemistry:*

1994-95	\$4.832 M
1995-96	\$4.780 M
1996-97	\$5.387 M
1997-98	\$5.542 M
1998-99	\$4.792 M
1999-00	\$5.418 M
2000-01	\$11.030 M
2001-02	\$8.302 M
2002-03	\$8.217 M

(Source: Data from the National Science Foundation HERD Report)

*Graduate Program (Changes during Term as Department Chair)*

Increased number of incoming Ph.D. students to 50-55 annually (from 35-40 annually)

*Safety Improvements (during Term as Department Chair)*

Installation of eyewash stations in the undergraduate teaching laboratories, for the first time

Installation of smoke detectors in the Chemistry building for the first time

Electrical renovations in the undergraduate teaching laboratories, to replace corroded and cracked electrical outlets

Enforcement of a policy requiring that students wear ANSI-standard goggles whenever working in the laboratory, and approved safety glasses whenever present in a laboratory where others are working

Acquisition of flame-proof storage cabinets for research laboratories; ventilation of storage cabinets

Upgrade in the ventilation of the lecture wing of the building, to permit lecture demonstrations to continue

Removal of Class A flammable solvents from sub-basement storage, bringing Department into code compliance

Removal of 1500 pounds of mercury from the building

Disposal of approximately 100 unlabeled lecture bottles of gases

Disposal of approximately 500 samples of inadequately labeled chemicals

Improvements in hazardous waste disposal; successful audits by Michigan Department of Environmental Quality

Establishment of laser safety guidelines

Monitoring of training-audit status

Perchloric acid hood demolition

Conversion of several stills to dry stills, in inorganic laboratories

\$8.7 million HVAC upgrade, to add approximately 75 new hoods to the building (up from 250)

*University Service*

MSU Interview Panel for Rhodes Scholarship Candidates (10/13/80-10/15/80, 10/13/81-10/15/81, 10/14/86-10/15/86, 10/15/87-10/16/87, 10/10/88-10/11/88, 10/9/89-10/10/89, 10/11/90, 10/4/91, 9/30/94, 9/29/95)

MSU Interview Panel for Marshall Scholarship Candidates (10/3/84-10/5/84, 9/25/92, 9/30/94, 9/7/18, 9/6/19, 9/11/20)

MSU Interview Panel for Churchill Fellowship Candidates (11/16/82-11/18/82, 11/96, 9/7/18, 9/6/19, 9/11/20)

MSU Interview Panel for Fulbright Fellowship Candidates (10/22/86, 10/14/87, 10/14/88, 10/19/88, 10/24/89, 10/22/90, 10/24/90, 10/24/91, 10/14/92, 10/19/92, 10/13/94-10/14/94, 9/27/95, 9/29/95, 10/2/95, 10/2/96, 10/4/96)

MSU Interview Panel for Truman Fellowship Candidates (2003)

MSU Alumni Distinguished Scholarship Selection Committee (1987-89, 2003)

Featherstone Scholarship Selection Committee (1996-2020)

MSU Chapter of Sigma Xi, Secretary (1991-93)

Referee for MSU AURI Grant proposals

Referee for MSU CFMR Grant proposals

Editorial Board, *The Centennial Review* (1/1/89-9/30/92)  
Search Committee, Vice President for Research and Graduate Studies (4/87-9/87), Vice-chair  
Search Committee, Dean of the College of Natural Science (7/95-3/96)  
Search Committee, Director of the Honors College (5/96-8/96)  
Search Committee, Director of the Lyman Briggs School (2002-03)

### ***Outreach and Student-oriented Activities***

Project supervisor for ACS Project SEED student, Laurie Page (Summer 1981)  
Project supervisor for MSU Professorial Assistants, Katherine Ahrens (1981-83), Paul Schreck  
(1982-83), Jason Wengert (2002-03), and Brian Wentzloff (2002-03)  
Research supervisor for NSF Research Experience for Undergraduates students, Sean Burns  
(Summer 1992), Kara Johnson (Summer 1993), and Rose Cory (Summer 1997)  
Research supervisor for GE Foundation Summer Research Student, Catherine Tloczynski  
(Summer 1992)  
Research supervisor for McNair Summer Research Opportunity Student, Suzanne Manjula Samuel  
(Summer 1998)  
Coach, Kinawa Middle School Science Olympiad Team, for the events Metric Estimation, Reach  
for the Stars, and Water Quality, 2001-03. Team placed first overall in regional competition in 2003,  
with first place in Reach for the Stars and Water Quality; fourth place statewide in Reach for the  
Stars, 2003  
Speaker, Science Day '88 (10/22/88); lecture entitled "Chemical Reactions: Entropy, Oscillations and  
Chaos" accompanied by demonstrations of the "Traffic Light" reaction, the "Old Nassau" reaction, the  
oscillating mercury drop, the Belousov-Zhabotinskii reaction, and the Briggs-Rauscher oscillating  
reaction  
Speaker, orientation session for MSU undergraduates applying for national fellowships  
(9/25/81, 9/23/82, 9/21/83, 9/17/84, 9/28/86, 9/23/87, 9/21/88, 6/1/89, 5/23/91, 5/28/92, 4/28/93,  
4/18/95, 4/18/97)  
Speaker, meeting of faculty and student participants in the College of Natural Science Mentor Program  
(4/7/91)  
Speaker, dinner for Alumni Distinguished Scholarship Competitors (2/22/80)  
Speaker, Phi Beta Kappa induction, "charge to new members" (5/24/88)  
Speaker, Emerging Scholars Program, Department of Mathematics (4/19/96)  
Guest lecturer, NSC 390H, "Measurement in Quantum Mechanics" (1/28/85)  
Author, university recruitment letter directed to honors-caliber undergraduates interested in natural science  
Academic advisor (~12 students annually, 1979-1998)  
Honors academic advisor (~15 students, 1979-1998)  
Academic advisor for MSU/University of Surrey exchange students in chemistry (4 students)

### ***Workshops and Discussion Panels***

Speaker, Big Ten Honors Programs Conference, Session on National Scholarships and Fellowships, (5/20/03)  
Workshop Presenter, "Out of the Lab, into Leadership," Michigan ACE Women's Network, Aspire Higher  
Conference (6/11/02)  
Panelist, Session on "Mentoring and Being Mentored," CIC Women in Science and Engineering Conference  
(11/7/98)  
Workshop Presenter, Great Lakes College Chemistry Conference Career Day, Michigan State University  
(10/5/96)  
Panelist, Lansing Area Meeting of the Association of Women in Science (4/17/91)  
Panelist, Discussion on "Women in Science," Lyman Briggs School (2/18/87)  
Panelist, Session on Research and Scholarly Activity, Conference on "How to Survive and Thrive in the  
MSU Academic Personnel System," Michigan State University (10/24/86)  
Panelist, Conference on "Growth and Survival: Women Graduates and Professionals in Progress,"  
Michigan State University (4/7/84)  
Panelist, Group of Women Chairs and Directors, Michigan State University NSF-Sponsored ADAPP Program,  
(Advancing Diversity through Alignment of Policies and Practices), Spring 2010

### ***National Professional Service***

Marshall Scholarship Selection Committee for the Chicago Consular Region (appointed by British Consul General in Chicago), 1997-2010; Chair, 2008-2016

Chair, Study of Gender Equity in the Marshall Scholarship Program (appointed by the British Ambassador to the United States, Sir Nigel Sheinwald), 2009-2016

Association of Marshall Scholars, Honorary Board Member, 2017

Councilor for Physical Chemistry, American Chemical Society, 1995-97

Chair, Midwest Chemistry Chairs' Group, 2000-02

Member, Committee of Visitors (triennial review of division), Chemistry Division, National Science Foundation, 3/4/98-3/6/98

Panelist, SBIR Program, Chemistry Division, National Science Foundation

Panelist, SBIR Program, Chemistry Division, National Science Foundation

Panelist, Chemistry 3 (Physical Chemistry), International Science Foundation, Panel to recommend funding for proposals from scientists in the former Soviet Union

Panelist, Graduate Research Traineeship Program, Panel to evaluate departmental proposals, Chemistry Division, National Science Foundation

Panelist, Presidential Young Investigator Award Review Panel, Chemistry Division, National Science Foundation

Chair, Michigan State University Section of the American Chemical Society, 1986-87

Chair, Conference Organizing Committee, Midwest Theoretical Chemistry Conference XXV, Michigan State University, 6/4/92-6/6/92

Session Chair, Fifteenth Annual Midwest Theoretical Chemistry Conference, 4/30/82-5/1/82

Session Chair, Midwest Theoretical Chemistry Conference, Northwestern University, 6/15/2014-6/17/2014

Session Chair, Midwest Theoretical Chemistry Conference, University of Michigan, 6/26/2015-6/28/2015

Session Chair, Midwest Theoretical Chemistry Conference, University of Pittsburgh, 6/9/2016-6/11/2016

Session Chair, Midwest Theoretical Chemistry Conference, Michigan State University, 6/1/2017-6/3/2017

Session Chair, Midwest Theoretical Chemistry Conference, University of Chicago, 6/21/2018-6/23/2018

Poster Session Judge, Midwest Theoretical Chemistry Conference, University of Illinois, 5/29/2013-5/31/2013

Poster Session Judge, Midwest Theoretical Chemistry Conference, University of Michigan, 6/26/2015-6/28/2015

Poster Session Judge, Midwest Theoretical Chemistry Conference, University of Pittsburgh, 6/9/2016-6/11/2016

Session Chair, Conference on Intermolecular Interactions: New Challenges for *ab initio* Theory, Telluride Scientific Research Center, Telluride, CO, 7/6/2015.

Session Chair, Telluride Conference on Intermolecular Interactions: New Challenges for *ab initio* Theory, Arenas de Cabrales, Spain, 7/8/2017-7/13/2017.

Session Chair, Conference on Intermolecular Interactions: New Challenges for *ab initio* Theory, Telluride Scientific Research Center, Telluride, CO, 3/19/2019.

External Reviewer, Department of Chemistry, Indiana University

External Reviewer, Department of Chemistry, University of Texas, San Antonio, proposal to establish Ph.D. program in Chemistry (committee of two, with Professor Martin Grubele, UIUC)

Referee for the *Journal of Chemical Physics*, *The Journal of Physical Chemistry*, *The Journal of Physical Chemistry Letters*, *The Journal of Chemical Education*, *Chemical Physics Letters*, *Chemical Physics*, *Molecular Physics*, *The Canadian Journal of Chemistry*, *The International Journal of Quantum Chemistry*, *The Journal of Statistical Physics*, *Physical Chemistry Chemical Physics*, *Theoretical Chemistry Accounts*, *The Journal of the American Chemical Society*, and *Physical Review Letters*

Referee for American Chemical Society/Petroleum Research Fund Proposals

Referee for Research Corporation, Cottrell Scholars

Referee for U. S. Department of Energy Proposals

Referee and Panelist for National Science Foundation Proposals