

## Publications of Katharine L. C. Hunt

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. 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, submitted to the *Proceedings of the Seventh International Conference of Computational Methods in Science and Engineering*, edited by George Maroulis and Theodore Simos (American Institute of Physics, College Park, Maryland, 2011).
73. 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).
74. 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).
75. 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).
76. 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*, accepted 8/7/2011.
77. 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 HTi<sup>0,+</sup>, *J. Chem. Phys.*, accepted 9/12/2011.
78. 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, submitted to *J. Chem. Phys.* 9/20/2011.
79. 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>, submitted to *J. Chem. Phys.* 9/20/2011.