

Publications of Giacinto Scoles

1. Boato, G.; Scoles, G.; Vallauri, M. E. Vapour Pressure of Isotopic Liquids I. *Nuovo Cimento* **1959**, *14*, 735–747.
2. Boato, G.; Casanova, G.; Scoles, G.; Vallauri, M. E. Vapour Pressure of Isotopic Liquids II. *Nuovo Cimento* **1961**, *20*, 87–93.
3. Boato, G.; Scoles, G.; Vallauri, M. E. Vapour Pressure of Isotopic Solids by a Steady Flow Method. *Nuovo Cimento* **1962**, *23*, 1041–1053.
4. Beenakker, J. J. M.; Scoles, G.; Knaap, H. F. P.; Jonkman, R. M. The Influence of a Magnetic Field on the Transport Properties of Diatomic Molecules in the Gaseous State. *Phys. Lett.* **1962**, *2*, 5–6.
5. Casanova, G.; Dondi, M. G.; Klein, M. L.; Scoles, G. Isotope Effects in Physical Adsorption and the Interaction Between Argon Atoms and Graphitized Carbon Blacks. *Discuss. Faraday Soc.* **1965**, *40*, 188–195.
6. Beenakker, J. J. M.; Hulsman, H.; Knaap, H. F. P.; Korving, J.; Scoles, G. The Influence of a Magnetic Field on the Viscosity and Other Transport Properties of Gaseous Diatomic Molecules. In *Advances in Thermophysical Properties at Extreme Temperatures and Pressures*; Gratch, S., Ed.; American Society of Mechanical Engineers: New York, 1965; pp 216–220.
7. Scoles, G.; van den Meijdenberg, C. J. N.; Bredewout, J. W.; Beenakker, J. J. M. Cryopump Techniques for Molecular Beam Experiments. *Physica* **1965**, *31*, 223–236.
8. Casanova, G.; Dondi, M. G.; Scoles, G.; Klein, M. L. Isotope Separation in Physical Adsorption. In *Fundamentals of Gas–Surface Interactions*; Staltsburg, H., Smith, J. N., Jr., Rogers, M., Eds.; Academic Press: New York, 1967; pp 258–270.
9. Cavallini, M.; Gallinaro, G.; Scoles, G. High Sensitivity Bolometer Detector for Molecular Beams. *Z. Naturforsch., A: Astrophys., Phys. Phys. Chem.* **1967**, *22*, 413–414.
10. Gallinaro, G.; Meneghetti, G.; Scoles, G. Visolectric Effect in Polar Polyatomic Gases. *Phys. Lett. A* **1967**, *24*, 451–452.
11. Korving, J.; Hulsman, H.; Knaap, H.; Beenakker, J. J. M.; Scoles, G. The Influence of a Magnetic Field on the Transport Properties of Gases of Polyatomic Molecules. *Physica* **1967**, *36*, 177–214.
12. Torello, F.; Scoles, G. Supersonic Molecular Beams Production and Temperature Distribution in Free Expanding Jets. *Meccanica* **1968**, *3*, 20–27.
13. Cantini, P.; Cavallini, M.; Dondi, M. G.; Scoles, G. Absolute Total Collision Cross Sections for Maxwellian Beams of Hydrogen and Helium Scattered by Room Temperature Hydrogen and Helium. *Phys. Lett. A* **1968**, *27*, 284–285.
14. Gazzola, G.; Scoles, G.; Torello, F. Temperature Distribution in Free Expanding Jets. In *VI International Symposium on Rarefield Gas Dynamics*; Trilling, L., Wachman, H. F., Eds.; Academic Press: New York, 1969; Vol. 2, pp 977–983.
15. Cavallini, M.; Gallinaro, G.; Scoles, G. A Superconducting Bolometer as a High Sensitivity Detector for Molecular Beams. *Z. Naturforsch., A: Astrophys., Phys. Phys. Chem.* **1969**, *24*, 1850–1851.
16. Dondi, M. G.; Torello, F.; Pauly, H.; Scoles, G. Energy Dependence on the Elastic Total Collision Cross Section of Identical Molecules: ${}^4\text{He}$. *J. Chem. Phys.* **1969**, *51*, 392–397.
17. Tommasini, F.; Levi, A. C.; Scoles, G.; deGroot, J. J.; van den Broeke, J. W.; van den Meijdenberg, C. J.; Beenakker, J. J. M. Viscosity and Thermal Conductivity of Polar Gases in an Electric Field. *Physica* **1970**, *49*, 299–341.
18. Levi, A. C.; Scoles, G.; Tommasini, F. Viscosity in an Electric Field of Mixtures of Polar Gases with Argon and Helium. *Z. Naturforsch., A: Astrophys., Phys. Phys. Chem.* **1970**, *25*, 1213–1219.
19. Cavallini, M.; Meneghetti, L.; Scoles, G.; Yealland, M. Differential Collision Cross Section Measurements in the Elastic Scattering of Light Identical Molecules: Helium. *Phys. Rev. Lett.* **1970**, *24*, 1469–1471.
20. Cavallini, M.; Gallinaro, G.; Meneghetti, L.; Scoles, G.; Valbusa, U. Rainbow Scattering and the Intermolecular Potential of Argon. *Chem. Phys. Lett.* **1970**, *7*, 303–305.
21. Tommasini, F.; Levi, A. C.; Scoles, G. Viscosity of Ammonia and Its Mixtures with Noble Gases in an Electric Field. *Z. Naturforsch., A: Astrophys., Phys. Phys. Chem.* **1971**, *26*, 1098–1100.
22. Cavallini, M.; Meneghetti, L.; Scoles, G.; Yealland, M. A Molecular Beam Scattering Apparatus with a Low Temperature Bolometer Detector. *Rev. Sci. Instrum.* **1971**, *42*, 1759–1763.
23. Cavallini, M.; Dondi, M. G.; Scoles, G.; Valbusa, U. Crossed Beams Measurements of the Differential Collision Cross Section of Heavy Rare Gases: Ar and Kr. *Entropie* **1971**, *42*, 136–139.
24. Cavallini, M.; Dondi, M. G.; Scoles, G.; Valbusa, U. Nonspherical Potentials and Molecular Scattering at Thermal Energies: N_2 and the Noble Gases. *Chem. Phys. Lett.* **1971**, *10*, 22–24.
25. Cantini, P.; Dondi, M. G.; Torello, F.; Scoles, G. Low Energy Repulsive Interaction Potential for Helium. *J. Chem. Phys.* **1972**, *56*, 1946–1956.
26. Dondi, M. G.; Valbusa, U.; Scoles, G. Energy Dependence of the Differential Collision Cross Section of H_2 at Thermal Energies. *Chem. Phys. Lett.* **1972**, *17*, 137–141.
27. Schutte, A.; Bassi, D.; Tommasini, F.; Scoles, G. Orbiting Resonances in the Scattering of H Atoms by Hg at Thermal Energies. *Phys. Rev. Lett.* **1972**, *29*, 979–982.
28. Marenco, G.; Schutte, A.; Scoles, G.; Tommasini, F. Interaction of Atomic and Molecular Hydrogen Beams with Surfaces at Very Low Temperatures. *J. Vac. Sci. Technol.* **1972**, *9*, 824–827.
29. Buck, U.; Dondi, M. G.; Valbusa, U.; Klein, M. L.; Scoles, G. Determination of the Interatomic Potential of Krypton. *Phys. Rev.* **1973**, *8*, 2409–2416.

30. Scoles, G. Quantum Symmetry Effects in the Scattering of Neutral Particles. In *The Physics of Electronic and Atomic Collisions*; Cobic, B., Kurepa, M. V., Eds.; Beograd: Yugoslavia, 1973; pp 583–594.
31. Bickes, R. W., Jr.; Este, G. O.; Scoles, G.; Smith, K. M. Molecular Beam Differential Collision Cross Section Measurements with H₂O. *J. Phys. B: At., Mol. Opt. Phys.* **1974**, *7*, L19–L21.
32. Scoles, G. Chemical Reactions Occurring at the Gas–Solid Interface. In *Dynamic Aspects of Surface Physics*; Goodman, F.O., Ed.; Editrice Compositori: Bologna, Italy, 1974; pp 588–604.
33. Este, G.O.; Hilko, B.; Swayer, D.; Scoles, G. New Compact Molecular Beam Velocity Selector. *Rev. Sci. Instrum.* **1975**, *46*, 223–225.
34. Schutte, A.; Bassi, D.; Tommasini, F.; Scoles, G. Energy Dependence of High Resolution Integral Collision Cross Section Measurements for Elastic Scattering of H and D Atoms by Hg at Thermal Energies. *J. Chem. Phys.* **1975**, *62*, 600–605.
35. Bickes, R. W., Jr.; Smith, K. M.; Scoles, G. Study of the Intermolecular Potentials for Hydrogen–Noble Gas Pairs via Molecular Beam Differential Scattering Measurements. *Can. J. Phys.* **1975**, *53*, 435–444.
36. Smith, K. M.; Rulis, A. M.; Scoles, G.; Aziz, R. A.; Duquette, G. Intermolecular Forces in Gaseous Mixtures: He–Ar. *J. Chem. Phys.* **1975**, *63*, 2250–2252.
37. Hepburn, J.; Penco, R.; Scoles, G. A Simple But Reliable Method for the Prediction of Intermolecular Potentials. *Chem. Phys. Lett.* **1975**, *36*, 451–455.
38. Bickes, R. W., Jr.; Duquette, G.; van den Meijdenberg, C. J. N.; Rulis, A. M.; Smith, K. M.; Scoles, G. Molecular Beam Scattering Experiments with Polar Molecules. *J. Phys. B: At., Mol. Opt. Phys.* **1975**, *8*, 3034–3043.
39. Schutte, A.; Bassi, D.; Tommasini, F.; Turelli, A.; Hermans, J. J. F.; Scoles, G. Recombination of Atomic Hydrogen on Low Temperature Surfaces. *J. Chem. Phys.* **1976**, *64*, 4135–4142.
40. Ahlrichs, R.; Penco, R.; Scoles, G. Intermolecular Forces in Simple Systems. *Chem. Phys.* **1977**, *19*, 119–130.
41. Smith, K. M.; Rulis, A. M.; Aziz, G. A.; Nain, V.; Scoles, G. Intermolecular Forces in Mixtures of He with the Heavier Noble Gases. *J. Chem. Phys.* **1977**, *67*, 152–163.
42. Gough, T. E.; Miller, R. E.; Scoles, G. Infrared Laser Spectroscopy of Molecular Beams. *Appl. Phys. Lett.* **1977**, *30*, 338–340.
43. Rulis, A. M.; Scoles, G. The Isotropic Part of the Potential Between Two H₂ Molecules. *Chem. Phys.* **1977**, *25*, 183–188.
44. Duquette, G.; Ellis, T. H.; Watts, R. O.; Klein, M. L.; Scoles, G. An Intermolecular Potential for (NH₃)₂. *J. Chem. Phys.* **1978**, *68*, 2544–2549.
45. Rulis, A. M.; Scoles, G.; Smith, K. M. Intermolecular Forces in Hydrogen–Noble Gas Mixtures. *Can. J. Phys.* **1978**, *56*, 753–762.
46. Este, G. O.; Knight, G.; Scoles, G. Scattering Experiments with Hydrogen Atoms. I. Differential Collision Cross Sections for H + Ar, D + Ar and H + CH₄. *Chem. Phys.* **1978**, *35*, 421–427.
47. Gough, T. E.; Miller, R.; Scoles, G. Sub-Doppler Resolution Infrared Spectroscopy of Supersonic Molecular Beams of NO. *J. Mol. Spectrosc.* **1978**, *72*, 124–127.
48. Gough, T. E.; Miller, R.; Scoles, G. Photoinduced Vibrational Predissociation of the van der Waals Molecule (N₂O)₂. *J. Chem. Phys.* **1978**, *69*, 1588–1590.
49. Gough, T. E.; Miller, R. E.; Scoles, G. Photoinduced Vibrational Predissociation of van der Waals Molecules. In *Advances in Laser Chemistry*; Spring Series in Chemical Physics 3; Zewail, A. H., Ed.; Springer-Verlag: New York, 1978; p 433.
50. Caracciolo, G.; Ellis, T. H.; Este, G. O.; Valbusa, U.; Ruffolo, A.; Scoles, G. Scattering Experiments with Hydrogen Atoms. II. A System of Astrophysical Interest: H + CO. *Astrophys. J.* **1979**, *229*, 451–454.
51. Aziz, R. A.; Riley, P. W.; Buck, U.; Maneke, G.; Schleusener, J.; Scoles, G.; Valbusa, U. On the Question of the Well Depth of the He–Ar Interatomic Potential. *J. Chem. Phys.* **1979**, *71*, 2637–2643.
52. Caracciolo, G.; Iannotta, S.; Scoles, G.; Valbusa, U. Diffractive Scattering of H Atoms from the (001) Surface of LiF at 78 K. *J. Chem. Phys.* **1980**, *72*, 4491–4499.
53. Govers, T. R.; Mattera, L.; Scoles, G. Molecular Beam Experiments on the Sticking and Accommodation of Molecular Hydrogen on a Low Temperature Substrate. *J. Chem. Phys.* **1980**, *72*, 5446–5455.
54. Scoles, G. Two-Body, Spherical, Atom–Atom and Atom–Molecule Interaction Energies. *Annu. Rev. Phys. Chem.* **1980**, *31*, 81–96.
55. Scoles, G. Intermolecular Forces: Hybrid Calculations. In *Proceedings of the Molecular Physics and Quantum Chemistry Workshop*; Wollongong, Australia, 1980.
56. Douketis, C.; Scoles, G.; Marchetti, S.; Zen, M.; Thakkar, A. Intermolecular Forces via Hybrid Hartree–Fock SCF Plus Damped Dispersion (HFD) Energy Calculations. An Improved Spherical Model. *J. Chem. Phys.* **1982**, *76*, 3057–3063.
57. Anderle, M.; Bassi, D.; Iannotta, S.; Marchetti, S.; Scoles, G. Measurement of the Spin Exchange Cross Section in the Collision of H Atoms with O₂ and NO by Means of Stored Atomic Beam Spectroscopy. *Phys. Rev. A: At., Mol., Opt. Phys.* **1981**, *23*, 34–35.
58. Bassi, D.; Boschetti, A.; Marchetti, S.; Scoles, G.; Zen, M. State Resolved Rotational Relaxation of CO in the Free Jet Expansion of He–CO Mixtures. *J. Chem. Phys.* **1981**, *74*, 2221–2227.
59. Ellis, T. H.; Iannotta, S.; Scoles, G.; Valbusa, U. High Resolution Diffractive Scattering of H and D Atoms by Single Crystal Surfaces. *J. Vac. Sci. Technol.* **1981**, *18*, 488–489.
60. Gough, T. E.; Miller, R. E.; Scoles, G. Sub-Doppler Resolution Infrared Molecular-Beam Spectroscopy. Stark-Effect Measurement of the Dipole Moment of Hydrogen Fluoride and Hydrogen Cyanide in Excited Vibrational State. *Faraday Discuss. Chem. Soc.* **1981**, *71*, 77–85.
61. Ellis, T. H.; Iannotta, S.; Scoles, G.; Valbusa, U. Diffractive Scattering of H Atoms from an Ordered Xenon Overlayer Adsorbed on the (001) Surface of Graphite. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1981**, *24*, 2307–2310.
62. Rodwell, W. R.; Scoles, G. Intermolecular Forces via Hybrid Hartree–Fock Plus Damped Dispersion (HFD) Energy Calculations. Systems with Small Nonsphericity: ArH₂, NeH₂ and HeH₂. *J. Phys. Chem.* **1982**, *86*, 1053–1059.

63. Gough, T. E.; Miller, R. E.; Scoles, G. The Infrared Spectra and Vibrational Predissociation of $(CO_2)_n$ Clusters Using Laser–Molecular Beam Techniques. *J. Phys. Chem.* **1981**, *85*, 4041.
64. Avrillier, S.; Raimond, J. M.; Bordé, Ch. J.; Bassi, D.; Scoles, G. Supersonic Beam Spectroscopy of Low J Transitions of the ν_3 Band of SF₆: Rabi Oscillations and Adiabatic Fast Passage with a c.w. Laser. *Opt. Commun.* **1981**, *39*, 311.
65. Bordé, Ch. J.; Avrillier, S.; van Lerberghe, A.; Salomon, Ch.; Bassi, D.; Scoles, G. Observation of Optical Ramsey Fringes in the 10 μm Spectral Region Using a Supersonic Beam of SF₆. *J. Phys.* **1981**, *42*, C8-15-19.
66. Ellis, T. H.; Scoles, G.; Valbusa, U. Bound State Resonant Scattering of Atoms from a Layer of Gas Absorbed on the Surface of a Crystal. *Surf. Sci.* **1982**, *118*, 1251–1256.
67. Gough, T. E.; Scoles, G. Optothermal Infrared Spectroscopy. In *Laser Spectroscopy V*; McKellar, A. R. W., Oka, T., Stoicheff, B., Eds.; Springer-Verlag: Berlin, 1981; p 337.
68. Bassi, D.; Boschetti, A.; Scoles, G.; Scotoni, M.; Zen, M. Infrared Multiple Photon Excitation of Sulfur Hexafluoride in a Molecular Beam. *Chem. Phys.* **1982**, *71*, 239–245.
69. Ellis, T. H.; Scoles, G.; Valbusa, U. Surface Vibrations of Atoms Physisorbed on a Crystal Surface: Monolayer and Bilayer Xenon on (0001) Graphite. *Chem. Phys. Lett.* **1983**, *94*, 247–249.
70. Gough, T. E.; Knight, D. G.; Scoles, G. Matrix Spectroscopy in the Gas Phase: IR Spectroscopy of Argon Clusters Containing SF₆ or CH₃F. *Chem. Phys. Lett.* **1983**, *97*, 155.
71. Gough, T. E.; Orr, B. J.; Scoles, G. Laser Stark Spectroscopy of Carbon Dioxide in a Molecular Beam. *J. Mol. Spectrosc.* **1983**, *99*, 143–158.
72. Este, G. O.; Knight, D. G.; Scoles, G.; Valbusa, U.; Grein, F. Interaction of Hydrogen Atoms with Polyatomic Molecules Studied by Means of Scattering Experiments and Hybrid Hartree–Fock Plus Damped Dispersion Calculations. *J. Phys. Chem.* **1983**, *87*, 2772–2780.
73. Jónsson, H.; Weare, J. H.; Ellis, T. H.; Scoles, G.; Valbusa, U. Atom-Scattering as a Quantitative Surface Probe: Noble Gas Monolayer and Bilayer on Graphite. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1984**, *30*, 4203.
74. Douketis, C.; Hutson, J. M.; Orr, B. J.; Scoles, G. Anisotropic Intermolecular Forces from Hartree–Fock Plus Damped Dispersion (HFD) Calculations. Application to Ar–HCl and Ar–HF. *Mol. Phys.* **1984**, *52*, 763.
75. Douketis, C.; Gough, T. E.; Scoles, G.; Wang, H. State Resolved Rotational Relaxation of CH₃F in the Free Jet Expansion of CH₃F–He Mixtures. *J. Phys. Chem.* **1984**, *88*, 4484–4487.
76. Bordé, Ch. J.; Salomon, Ch.; Avrillier, S.; van Lerberghe, A.; Breant, Ch.; Bassi, D.; Scoles, G. Optical Ramsey Fringes with Travelling Waves. *Phys. Rev. A: At., Mol., Opt. Phys.* **1984**, *A30*, 1836–1849.
77. Iannotta, S.; Scoles, G.; Valbusa, U. The Effects of Surface Atom Vibrations on the Diffraction of ¹H and ²H Beams from the Basal Plane of Graphite. *J. Phys. Chem.* **1985**, *89*, 1914–1921.
78. Ellis, T. H.; Scoles, G.; Valbusa, U.; Jónsson, H.; Weare, J. H. Hydrogen Atom Scattering from Physisorbed Overlayers. I. Diffraction. *Surf. Sci.* **1985**, *155*, 499–534.
79. Iannotta, S.; Scoles, G.; Valbusa, U. NaCl(001) Surface Study by H Atom Scattering. Part I: Diffraction. *Surf. Sci.* **1985**, *161*, 411.
80. Iannotta, S.; Scoles, G.; Valbusa, U. NaCl(001) Surface Study by H Atom Scattering. Part II: Bound State Resonances. *Surf. Sci.* **1985**, *161*, 429.
81. Adam, A. G.; Gough, T. E.; Isenor, N. R.; Scoles, G. Rabi Oscillations and Rapid Passage Effects in the Molecular Beam CO₂ Laser Stark Spectroscopy of CH₃F. *Phys. Rev. A: At., Mol., Opt. Phys.* **1985**, *33*, 1451.
82. Danielson, L.; Ruiz, J. C.; Schwartz, C.; Scoles, G.; Hutson, J. M. Very Low Energy Scattering of Helium Atoms from Crystal Surfaces. A Quantitative Comparison Between Experiment and Theory. *Faraday Discuss. Chem. Soc.* **1985**, *80*, 47.
83. Gough, T. E.; Mengel, M.; Rowntree, P. A.; Scoles, G. Infrared Spectroscopy at the Surface of Clusters. A New Type of Surface Spectroscopy: SF₆ on Ar. *J. Chem. Phys.* **1985**, *83*, 4958.
84. Buck, U.; Kohlhase, A.; Secret, D.; Phillips, T.; Scoles, G.; Grein, F. Rotationally Inelastic Scattering and Potential Calculations for Ne + CH₄. *Mol. Phys.* **1985**, *85*, 1233.
85. Gough, T. E.; Knight, D. G.; Rowntree, P. A.; Scoles, G. Molecular Beam Infrared Photodissociation of van der Waals Molecules Containing SF₆. *J. Phys. Chem.* **1986**, *90*, 4026.
86. Adam, A. G.; Gough, T. E.; Isenor, N. R.; Scoles, G.; Shelley, J. The Observation of Two Zone Ramsey Fringes Using Laser Stark Spectroscopy of a Molecular Beam. *Phys. Rev. A: At., Mol., Opt. Phys.* **1986**, *34*, 4803.
87. Cai, W. Q.; Gough, T. E.; Gu, X. J.; Isenor, N. R.; Scoles, G. Transition Dipole Moment Measurements for the ν_2 Band of NH₃ with Molecular Beam Laser Stark Spectroscopy. *J. Mol. Spectrosc.* **1986**, *120*, 374–380.
88. Ruiz, J. C.; Jónsson, H.; Scoles, G. On the Laterally Averaged Interaction Potential between He Atoms and the (0001) Surface of Graphite. *Chem. Phys. Lett.* **1986**, *129*, 139.
89. Gough, T. E.; Gu, X. J.; Isenor, N. R.; Scoles, G. Transition Dipole Moment for the C–O Stretching Band of CH₃OH Measured with Molecular Beam Laser Stark Spectroscopy. *Int. J. Infrared Millimeter Waves* **1986**, *7*, 1893–1901.
90. Jónsson, H.; Weare, J. H.; Ellis, T. H.; Scoles, G. Hydrogen Atom Scattering from Physisorbed Overlays. II. A Different Kind of Resonance Crossing. *Surf. Sci.* **1987**, *180*, 353–370.
91. Cai, W. Q.; Gough, T. E.; Gu, X. J.; Isenor, N. R.; Scoles, G. Polarizability of CO₂ Studied in Molecular Beam Laser Stark Spectroscopy. *Phys. Rev. A: At., Mol., Opt. Phys.* **1987**, *36*, 4722–4727.
92. Levandier, D.; Pursel, R.; Scoles, G. Complex Forming Reactions in Noble Gas Clusters. In *Proceedings of the NATO Workshop on van der Waals Clusters*, Maratea, Italy, Sept 22–26, 1986; Weber, A. Ed.

93. Gough, T. E.; Mengel, M.; Rountree, P.; Scoles, G. Molecular Spectroscopy in and on Noble Gas Clusters. In *Laser Applications in Chemistry*; Evans, D. K., Ed.; Proceedings of SPIE—the International Society for Optical Engineering 669; SPIE—the International Society for Optical Engineering: Bellingham, WA, 1986; pp 129–132.
94. Levandier, D. J.; McCombie, J.; Pursel, R.; Scoles, G. Complex-Forming Reactions in Neutral Noble Gas Clusters. *J. Chem. Phys.* **1987**, *86*, 7239.
95. Ihm, G.; Cole, M. W.; Toigo, F.; Scoles, G. Systematic Trends in van der Waals Interactions: Atom–Atom and Atom–Surface Cases. *J. Chem. Phys.* **1987**, *87*, 3995–3999.
96. Scoles, G. Introduction. In *Atomic and Molecular Beam Methods*; Scoles, G., Bassi, D., Buck, U., Lainé, D., Eds.; Oxford University Press: New York, 1988; Chapter 1, pp 3–13.
97. Ruiz, J. C.; Klein, M. L.; Moller, M. A.; Rountree, P.; Scoles, G.; Xu, J. Structure of Physisorbed Overlays of Dipolar Molecules: A Combined Study by Atomic Beam Scattering and Molecular Dynamics. *Phys. Rev. Lett.* **1988**, *61*, 710.
98. Scoles, G. Chemical Dynamics in Systems of Finite Size. In *Workshop on Molecular and Cluster Beam Science*; National Academy Press: Washington, DC, 1988; pp 46–56.
99. Gu, X. J.; Isenor, N. R.; Scoles, G. On the Vibrational State-Dependent Polarizability of CO₂. *Phys. Rev. A: At., Mol., Opt. Phys.* **1989**, *39*, 413.
100. Levandier, D. J.; Mengel, M.; Pursel, R.; McCombie, J.; Scoles, G. Molecular Beam Infrared Spectroscopy and Complex-Forming Reactions of CH₃F in Argon Clusters. *Z. Phys. D: At., Mol. Clusters* **1988**, *10*, 337.
101. Zhang, B.; Gu, X.; Isenor, N. R.; Scoles, G. Transition Dipole Moment Measurements for the ν₉ Band of Difluoromethane Using Rabi Oscillations. *Chem. Phys.* **1988**, *126*, 151.
102. Levandier, D. J.; Mengel, M.; Scoles, G. Infrared Spectroscopy in and on Argon Clusters: Surface and Matrix Spectroscopy in the Gas Phase. In *The Chemical Physics of Atomic and Molecular Clusters*, Proceedings of the International School of Physics “Enrico Fermi”, Course 107, Varenna, Italy, June 28–July 7, 1988; North-Holland: New York, 1990; p 331.
103. Meyer, H.; Kerstel, E. R.Th.; Zhuang, D.; Scoles, G. Sub-Doppler Rotationally Resolved Overtone Spectroscopy of the HCN Dimer. *J. Chem. Phys.* **1989**, *90*, 4623.
104. McCombie, J.; Scoles, G. Molecular Collisions in, with and on Clusters. In *XVI ICPEAC*; Dalgarno, A., et al., Eds.; AIP Conference Proceedings 205; American Institute of Physics: New York, 1990; pp 430–441.
105. Rountree, P.; Scoles, G.; Xu, J. Low Energy Helium Atom Scattering from HCl Monolayers Physisorbed on Graphite. *Surf. Sci.* **1989**, *224*, 43.
106. Chidsey, C. E. D.; Liu, G.-Y.; Rountree, P.; Scoles, G. Molecular Order at the Surface of an Organic Monolayer Studied by Low Energy Helium Diffraction. *J. Chem. Phys.* **1989**, *91*, 4421.
107. Liu, G.Y.; Rountree, P.; Scoles, G.; Xu, J. The Structure of Ammonia Overlays Physisorbed onto the Surface of Single Crystal Graphite, Determined by Means of Atomic Beam Diffraction. *J. Chem. Phys.* **1990**, *92*, 3853.
108. Aziz, R. A.; Buck, U.; Jónsson, H.; Ruiz-Suaréz, J. C.; Schmidt, B.; Scoles, G.; Slaman, M. J.; Xu, J. Two and ThreeBody Forces in the Interaction of He Atoms with Xe Overlays Adsorbed on (0001) Graphite. *J. Chem. Phys.* **1989**, *91*, 6477.
109. Levandier, D. J.; Goyal, S.; McCombie, J.; Pate, B.; Scoles, G. Infrared Spectroscopy and Dimer Formation at the Surface of Medium–Large Argon Clusters. *J. Chem. Soc., Faraday Trans.* **1990**, *86*, 2361.
110. Rountree, P. A.; Ruiz-Suaréz, J. C.; Scoles, G. Low Energy Helium Scattering from Ordered Physisorbed Layers of Polar Molecules. *J. Phys. Chem.* **1990**, *94*, 8511–8522.
111. Gu, X. J.; Levandier, D. J.; Zhang, B.; Scoles, G.; Zhuang, D. On the IR Spectroscopy of SiF₄ and SF₆ in Ar Clusters. Location of the Solute. *J. Chem. Phys.* **1990**, *93*, 4898–4906.
112. Liu, G.-Y.; Scoles, G.; Wang, J. He Diffraction from Overlays Physisorbed in a Self-Assembled Organic Monolayer. *Langmuir* **1990**, *6*, 1804–1806.
113. Lehmann, K. K.; Pate, B. H.; Scoles, G. Eigenstate resolved ν₁ Spectrum of CF₃CCH: Anharmonic Couplings to the Bath. *J. Chem. Soc., Faraday Trans.* **1990**, *86*, 2071.
114. Scoles, G. On the Prediction of Intermolecular Forces between Unlike Atoms and Molecules. *Int. J. Quantum Chem.: Quantum Chem. Symp.* **1990**, *24*, 475–479.
115. Lehmann, K. K.; Pate, B. H.; Scoles, G. Statistical IVR and Its Hindrance: The Fundamentals of (CH₃)₃CCCH and (CH₃)₃SiCCH. *J. Chem. Phys.* **1990**, *93*, 2152.
116. Scoles, G. Thermal Detection Laser Spectroscopy of Molecular Beams. In *Proceedings of the Conference on Lasers in Chemistry*, Trieste, Italy, June 1990; Proceedings – Indian Academy of Sciences, Chemical Sciences 103 (3); 1991.
117. Ruiz-Suarez, J. C.; Vargas, M. C.; Goodman, F. O.; Scoles, G. Zero Order Desorption of Xe from (0001) Graphite: An Experimental Study and a Theoretical Model. *Surf. Sci.* **1991**, *243*, 219–226.
118. Goyal, S.; Robinson, G. N.; Schutt, D. L.; Scoles, G. Infrared Spectroscopy of SF₆ in and on Argon Clusters in an Extended Range of Cluster Sizes: Finite-Size Particles Attaining Bulk-like Properties. *J. Phys. Chem.* **1991**, *95*, 4186.
119. Kerstel, E.; Lehmann, K. K.; Mentel, T. F.; Pate, B. H.; Scoles, G. Dependence of Intramolecular Vibrational Relaxation on Central Atom Substitution: The ν₁ and 2ν₁ Molecular Beam Optothermal Spectra of (CH₃)₃C—C≡C—H and (CH₃)₃Si—C≡C—H. *J. Phys. Chem.* **1991**, *95*, 8282.
120. Pate, B. H.; Lehmann, K. K.; Scoles, G. The Onset of Intramolecular Vibrational Energy Redistribution and its Intermediate Case: The ν₁ and 2ν₁ Molecular Beam Optothermal Spectra of Trifluoropropyne. *J. Chem. Phys.* **1991**, *95*, 3891.
121. Camillone, N., III.; Chidsey, C. E. D.; Liu, G. Y.; Putvinski, T. M.; Scoles, G. Surface Structure and Thermal Motion of n-Alkane Thiols Self-Assembled on Au(111), Studied by Low Energy Helium Diffraction. *J. Chem. Phys.* **1991**, *94*, 8493.
122. Hovde, D. C.; Timmermans, J. H.; Scoles, G.; Lehmann, K. K. High Power Injection Seeded Optical Parametric Oscillator. *Opt. Commun.* **1991**, *86*, 294–300.

123. Fenter, P.; Eisenberger, P.; Li, J.; Camillone, N., III.; Bernasek, S.; Scoles, G.; Ramanarayanan, T. A.; Liang, K. S. The Structure of $\text{CH}_3(\text{CH}_2)_{17}\text{SH}$ Self-Assembled on the Ag(111) Surface: An Incommensurate Monolayer. *Langmuir* **1991**, *7*, 2013.
124. Lehmann, K. K.; Pate, B. H.; Scoles, G. On the Measurement of the Rate of Intramolecular Vibrational Energy Redistribution via High Resolution Molecular Beam Optothermal Spectroscopy. In *Laser Chemistry II*; 1991; pp 237–245.
125. Lehmann, K. K.; Pate, B. H.; Scoles, G. Intramolecular Vibrational Redistribution on the Nanosecond Timescale: ν_1 and $2\nu_1$ Spectra of Substituted Acetylene Compounds. In *Mode Selective Chemistry*; Jortner, J., Levine, R. D., Pullman, B., Eds.; Kluwer Academic Publishers: Dordrecht, The Netherlands, 1991; pp 17–23.
126. Liu, G. Y.; Robinson, G. N.; Scoles, G.; Heiney, P. Low Energy Helium Diffraction Studies of CO_2 Overlays Physisorbed on NaCl (001). *Surf. Sci.* **1992**, *262*, 409–421.
127. Robinson, G. N.; Camillone, N., III.; Rowntree, P. A.; Liu, G. Y.; Wang, J.; Scoles, G. Low Energy Helium Diffraction Studies of CH_3Br Overlays Physisorbed on C(0001), NaCl(001) and LiF (001) Surfaces. *J. Chem. Phys.* **1992**, *96*, 9212.
128. Goyal, S.; Schutt, D.L.; Scoles, G. Infrared Spectroscopy of SF_6 Attached to Classical and Quantum Clusters. In *Proceedings of the NATO Conference: From Clusters to Crystals*, Richmond, VA, Oct 8–12, 1991.
129. Goyal, S.; Schutt, D. L.; Scoles, G. Vibrational Spectroscopy of SF_6 Attached to He Clusters. *Phys. Rev. Lett.* **1992**, *69*, 933.
130. Gambogi, J. E.; L'Esperance, R. P.; Lehmann, K. K.; Pate, B. H.; Scoles, G. Influence of Methyl Group Deuteration on the Rate of Intramolecular Vibrational Energy Relaxation. *J. Chem. Phys.* **1993**, *98* (2), 1116–1122.
131. Kerstel, E. R. Th.; Meyer, H.; Lehmann, K. K.; Scoles, G. The Rotationally Resolved $1.5 \mu\text{m}$ Spectrum of the HCN–HF Hydrogen Bonded Complex. *J. Chem. Phys.* **1992**, *97*, 8896.
132. Goyal, S.; Schutt, D. L.; Scoles, G. The Infrared Spectrum of SF_6 Solvated in Large Molecular H_2 Clusters. *Chem. Phys. Lett.* **1992**, *196*, 123.
133. Camillone, N., III.; Chidsey, C. E. D.; Liu, G. Y.; Scoles, G. Superlattice Structure at the Surface of a Monolayer of Octadecanethiol Self-Assembled on Au(111). *J. Chem. Phys.* **1993**, *98* (4), 3503–3511.
134. Gambogi, J. E.; Lehmann, K. K.; Pate, B. H.; Scoles, G.; Yang, X. The Rate of Intramolecular Vibrational Energy Relaxation of the Fundamental C–H Stretch in $(\text{CF}_3)_3\text{C}\equiv\text{C}-\text{H}$. *J. Chem. Phys.* **1993**, *98* (2), 1748–1749.
135. Camillone, N., III.; Chidsey, C. E. D.; Liu, G. Y.; Scoles, G. Substrate Dependence of the Surface Structure and Chain Packing of Docosyl Mercaptan Self-Assembled on the (111), (110), and (100) Faces of Single Crystal Gold. *J. Chem. Phys.* **1993**, *98* (5), 4234–4245.
136. Goyal, S.; Schutt, D. L.; Scoles, G. Molecular Solvation in Atomic Clusters Studied by Means of Molecular Beam Infrared Spectroscopy. *Acc. Chem. Res.* **1993**, *26*, 123–130.
137. Lehmann, K. K.; Pate, B. H.; Scoles, G. Intramolecular Vibrational Relaxation in Large Molecules: Homogeneous Lifetimes and the Mechanism of Energy Relaxation. In *From Molecular Dynamics to Combustion Chemistry*; Carra, S., Rahman, N., Eds.; World Scientific: 1992.
138. Dolce, J. W.; Yang, B.; Saeed, M.; DiMauro, L.; Scoles, G. Highly Efficient Synchronous Amplification of a Picosecond Dye Laser at a Kilohertz Repetition Rate. *Appl. Phys. B: Photophys. Laser Chem.* **1993**, *56*, 43–46.
139. Kerstel, E. R. Th.; Scoles, G.; Yang, X. Structure and Predissociation Dynamics of $(\text{HCCN})_2$: A High Resolution IR Study. *J. Chem. Phys.* **1993**, *99*, 876–884.
140. Yang, X.; Kerstel, E. R. Th.; Scoles, G. Intramolecular Coupling Enhanced Predissociation in HCCN–HCN. *J. Chem. Phys.* **1993**, *98*, 2727–2734.
141. Yang, X.; Pearson, R. Z.; Scoles, G. High Resolution IR Study of the NCCCH–CO complex. *Chem. Phys. Lett.* **1993**, *204*, 145–151.
142. Goyal, S.; Schutt, D. L.; Scoles, G. Infrared Spectroscopy in Highly Quantum Matrices: Vibrational Spectrum of $(\text{SF}_6)_{n=1,2}$ Attached to Helium Clusters. *J. Phys. Chem.* **1993**, *97*, 2236–2245.
143. Camillone, N., III.; Chidsey, C. E. D.; Eisenberger, P.; Fenter, P.; Li, J.; Liang, K. S.; Liu, G. Y.; Scoles, G. Structural Defects in Self-Assembled Organic Monolayers via Combined Atomic Beam and X-Ray Diffraction. *J. Chem. Phys.* **1993**, *99*, 744–747.
144. Yang, X.; Kerstel, E. R. Th.; Scoles, G. A High Resolution Infrared Study of HCCCN–HCN and HCCCN–HF. *J. Chem. Phys.* **1993**, *99* (1), 760–761.
145. Kerstel, E. R. Th.; Pate, B. H.; Mentel, Th. F.; Yang, X.; Scoles, G. Sub-Doppler Infrared Spectroscopy of HCCCN– BF_3 (ν_1) and HCN– BF_3 (ν_1 and $2\nu_1$). *J. Chem. Phys.* **1994**, *101* (4), 2762–2771.
146. Kerstel, E. R. Th.; Lehmann, K. K.; Gambogi, J. E.; Yang, X.; Scoles, G. The ν_1 Vibrational Predissociation Lifetime of $(\text{HCN})_2$ Determined from Upper State Microwave–Infrared Double Resonance. *J. Chem. Phys.* **1993**, *99*, 8559–8570.
147. Gambogi, J. E.; Timmermans, J. H.; Lehmann, K. K.; Scoles, G. Enhanced Instability of Extreme Motion States in Propyne: Lifetimes of Overtone Bands Versus Isoenergetic Combination States. *J. Chem. Phys.* **1993**, *99*, 9314–9317.
148. Kerstel, E. R. Th.; Lehmann, K. K.; Mentel, Th. F.; Scoles, G.; Timmermans, J. H. The Rotationally-Resolved $3 \mu\text{m}$ Spectrum and the Structure of the ICCH Dimer. *J. Mol. Spectrosc.* **1993**, *162*, 342–352.
149. Kerstel, E. R. Th.; Lehmann, K. K.; Pate, B. H.; Scoles, G. Reinvestigation of the Acetylene CH Stretching Fundamental of Propyne via High Resolution, Optothermal Infrared Spectroscopy: Non-resonant Perturbations to ν_1 . *J. Chem. Phys.* **1994**, *100*, 2588–2595.
150. McIlroy, A.; Nesbitt, D. J.; Kerstel, E. R. Th.; Pate, B. H.; Lehmann, K. K.; Scoles, G. Subdoppler, Infrared Laser Spectroscopy of the Propyne $2\nu_1$ Band: Evidence of z -Axis Coriolis Dominated Intramolecular State Mixing in the Acetylenic CH Stretch Overtone. *J. Chem. Phys.* **1994**, *100*, 2596–2611.

151. Gambogi, J. E.; Kerstel, E. R. Th.; Lehmann, K. K.; Scoles, G. Eigenstate Resolved Infrared–Infrared Double Resonance Spectroscopy of the $3\nu_1$ Band of Propyne: Intramolecular Vibrational Energy Redistribution into a Coriolis Coupled Bath. *J. Chem. Phys.* **1994**, *100*, 2612–2622.
152. Gambogi, J. E.; L’Esperance, R.; Lehmann, K. K.; Scoles, G. Long Range, Resonant Vibrational Energy Exchange in Polyatomic Molecules: The Fundamental Acetylenic CH Stretching Spectrum of $\text{CH}_3\text{Si}(\text{C}\equiv\text{CH})_3$. *J. Phys. Chem.* **1994**, *98*, 5614.
153. Lehmann, K. K.; Pate, B. H.; Scoles, G. Intramolecular Dynamics from Eigenstate-Resolved Infrared Spectra. *Annu. Rev. Phys. Chem.* **1994**, *45*, 241–274.
154. Camillone, N., III.; Leung, T. Y. B.; Scoles, G. Interactions and Structure of *n*-Alkane Thiol Monolayers on Gold Surfaces. In *Laser Techniques for Surface Science*; Dai, H.-L., Sibener, S. J., Eds.; Proceedings of SPIE—the International Society for Optical Engineering 2125; SPIE—the International Society for Optical Engineering: Bellingham, WA, 1994; pp 174–181.
155. Becucci, M.; Gambogi, J. E.; Timmermans, T. H.; Lehmann, K. K.; Scoles, G.; Gard, G. L.; Winter, R. Molecular Beam Infrared Spectroscopy and Intramolecular Dynamics of SF_5CCH in the Region of the Fundamental and First Overtone of the Acetylenic CH Stretch. *Chem. Phys.* **1994**, *187*, 11–19.
156. Amar, F. G.; Goyal, S.; Levandier, D. J.; Perera, L.; Scoles, G. IR Spectroscopy of Solvated Molecules. In *Clusters of Atoms and Molecules II: Solvation and Chemistry of Free Clusters, and Embedded, Supported, and Compressed Clusters*; Springer Series in Chemical Physics 56; Haberland, H., Ed.; Springer-Verlag: Berlin, 1994; Chapter 2.2.
157. Callegari, A.; DiLieto, A.; Minguzzi, P.; Tonelli, M.; Scoles, G.; Janssen, H. P. Spectroscopy of DCN in Molecular Beam Using a YLF Laser at $1.9 \mu\text{m}$. *J. Phys. IV* **1994**, *4*, C4-679–682.
158. Camillone, N., III.; Eisenberger, P.; Leung, T. Y. B.; Schwartz, P.; Scoles, G.; Poirier, G. E.; Tarlov, M. J. New Monolayer Phases of *n*-Alkane Thiols Self-Assembled on Au(111). Preparation, Surface Characterization and Imaging. *J. Chem. Phys.* **1994**, *101*, 11031.
159. Goyal, S.; Schutt, D. L.; Scoles, G. Noble Gas Clusters as Matrices for IR Spectroscopy. From Small Clusters to the Bulk-Matrix Limit: SF_6Ar_n , SF_6Kr_n and SF_6Xe_n with $100 < n < 10,000$. *J. Chem. Phys.* **1995**, *102* (6), 2302–2314.
160. Li, J.; Liang, K. S.; Camillone, N., III.; Leung, T. Y. B.; Scoles, G. The Structure of *n*-Octadecane Thiol Monolayers Self-Assembled on Au(001) Studied by Synchrotron X-ray and Helium Atom Diffraction. *J. Chem. Phys.* **1995**, *102* (12), 5012–5028.
161. Gambogi, J. E.; Becucci, M.; O’Brien, Ch.; Lehmann, K. K.; Scoles, G. Reinvestigation of the $2\nu_1$ Band of Trifluoropropyne Using a Frequency Stabilized $1.5 \mu\text{m}$ Color Center Laser in Conjunction with a Laser Field Build-up Cavity. *Ber. Bunsen-Ges.* **1995**, *99* (3), 548–554.
162. Stienkemeier, F.; Higgins, J.; Ernst, W. E.; Scoles, G. Laser Spectroscopy of Alkali-Doped Helium Clusters. *Phys. Rev. Lett.* **1995**, *74* (18), 3592–3595.
163. Gambogi, J. E.; Pearson, R. Z.; Yang, X.; Lehmann, K. K.; Scoles, G. Intramolecular Vibrational Dynamics of Diacetylene and Diacetylene- d_1 via Eigenstate-Resolved Overtone Spectroscopy. *Chem. Phys.* **1995**, *190*, 191–205.
164. Timmermans, W. H.; Lehmann, K. K.; Scoles, G. Intramolecular Dynamics of Allene in the Region around 6000 cm^{-1} via Eigenstate-Resolved IR Spectroscopy. *Chem. Phys.* **1995**, *190*, 393–405.
165. Stienkemeier, F.; Ernst, W. E.; Higgins, J.; Scoles, G. On the Use of Liquid He Cluster Beams for the Preparation and Spectroscopy of the Triplet States of Alkali Dimers and Other Weakly Bound Complexes. *J. Chem. Phys.* **1995**, *102* (1), 615–617.
166. Yang, X.; Kerstel, E. R. Th.; Scoles, G.; Bemish, R. J.; Miller, R. High Resolution Infrared Molecular Beam Spectroscopy of Cyanoacetylene Clusters. *J. Chem. Phys.* **1995**, *103* (20), 8828–8839.
167. Li, J.; Liang, K. S.; Scoles, G.; Ulman, A. Counterion Overlays at the Interface between an Electrolyte and an ω -Functionalized Monolayer Self-Assembled on Gold. An X-ray Reflectivity Study. *Langmuir* **1995**, *11*, 4418–4427.
168. Stienkemeier, F.; Higgins, J.; Ernst, W. E.; Scoles, G. Spectroscopy of Alkali Atoms and Molecules Attached to Liquid Helium Clusters. *Z. Phys. B: Condens. Matter* **1995**, *98*, 413–416.
169. Gambogi, J. E.; Kerstel, E. R. Th.; Yang, X. M.; Lehmann, K. K.; Scoles, G. High Resolution Spectrum of the $3\nu_1$ Band of Cyanoacetylene. *J. Mol. Spectrosc.* **1996**, *175*, 198–202.
170. Stienkemeier, F.; Higgins, J.; Ernst, W.; Callegari, C.; Scoles, G. Spectroscopy of Alkali Atoms and Molecules Attached to Highly Quantum Clusters. In *Laser Spectroscopy*, Proceedings of the XII International Conference, Capri, Italy; World Scientific: 1996; pp 377–381.
171. Camillone, N., III.; Leung, T. Y. B.; Schwartz, P.; Eisenberger, P.; Scoles, G. Chain Length Dependence of the Striped Phases of Alkanethiol Monolayers Self-Assembled on Au(111): An Atomic Beam Diffraction Study. *Langmuir* **1996**, *12*, 2737–2746.
172. Yang, X.; Pearson, R. Z.; Lehmann, K. K.; Scoles, G. Molecular Beam IR Spectroscopy of the $\text{HCCN}-\text{HCCH}$ and $\text{HCN}-\text{HCCCCH}$ van der Waals Complexes. *J. Chem. Phys.* **1996**, *105* (24), 10725–10733.
173. Yang, X.; Pearson, R. Z.; Scoles, G. A High Resolution IR study of the van der Waals Complexes of HCCCN with CO_2 and N_2 . *J. Mol. Spectrosc.* **1996**, *180*, 1–6.
174. Bemish, R. J.; Miller, R. E.; Yang, X.; Scoles, G. The Argon–Diacetylene Complex: An Example of Distributed Interactions and Transferable Potentials. *J. Chem. Phys.* **1996**, *105* (23), 10171–10177.
175. Higgins, J.; Callegari, C.; Reho, J.; Stienkemeier, F.; Ernst, W. E.; Lehmann, K. K.; Gutowski, M.; Scoles, G. Photoinduced Chemical Dynamics of High Spin Alkali Trimers. *Science* **1996**, *273*, 629–631.
176. Higgins, J.; Ernst, W. E.; Gutowski, M.; Callegari, C.; Reho, J.; Lehmann, K. K.; Scoles, G. Spin Polarized Alkali Clusters: Observation of Quartet States of the Sodium Trimer. *Phys. Rev. Lett.* **1996**, *77*, 4532.
177. Stienkemeier, F.; Higgins, J.; Callegari, C.; Ernst, W. E.; Kanorsky, S. I.; Scoles, G. Spectroscopy of Alkali Atoms (Li, Na, K) Attached to Large He Clusters. *Z. Phys. D: At., Mol. Clusters* **1996**, *38*, 253.

178. DeKieviet, M. F. M.; Bahatt, D.; Scoles, G.; Vidali, G.; Karimi, G. An Atomic Beam Diffraction Study of a Rare Gas Monolayer of Square Symmetry: Kr on (100) NaCl. *Surf. Sci.* **1996**, *365*, 789–800.
179. Camillone, N., III.; Leung, T. Y. B.; Scoles, G. A Low Energy He Atom Diffraction Study of Decanethiol Self-Assembled on Au(111). *Surf. Sci.* **1997**, *373* (2/3), 333–349.
180. Dolce, J. W.; Callegari, A.; Meyer, B.; Lehmann, K. K.; Scoles, G. Chromophore Dependence of Intramolecular Vibrational Redistribution: CH Stretch First Overtone vs. SiH Stretch Second Overtone in Methylsilane. *J. Chem. Phys.* **1997**, *107* (17), 6549.
181. Callegari, A.; Srivastava, H. K.; Merker, U.; Lehmann, K. K.; Scoles, G.; Davis, M. J. Eigenstate Resolved Infrared–Infrared Double Resonance Study of Intramolecular Vibrational Relaxation in Benzene: First Overtone of the CH Stretch. *J. Chem. Phys.* **1997**, *106* (1), 432–435.
182. Reho, J.; Callegari, C.; Higgins, J.; Ernst, W. E.; Lehmann, K. K.; Scoles, G. Spin-Orbit Effects in the Formation of the Na/He Excimer on the Surface of Helium Clusters. In *Dynamics of Electronically Excited States in Gaseous, Cluster and Condensed Media*; Faraday Discussions of the Chemical Society 108; Royal Society of Chemistry: London, 1998; pp 161–174.
183. Lavrich, D.; Wetterer, S.; Bernasek, S.; Scoles, G. Physisorption and Chemisorption of Alkanethiols and Alkyl Sulfides on Au(111). *J. Phys. Chem. B* **1998**, *102* (18), 3456–3465.
184. Wetterer, S.; Lavrich, D.; Cummings, T.; Bernasek, S.; Scoles, G. Energetics and Kinetics of the Physisorption of Hydrocarbons on Au(111). *J. Phys. Chem. B* **1998**, *102* (46), 9266–9275.
185. Callegari, C.; Higgins, J.; Stienkemeier, F.; Scoles, G. Beam Depletion Spectroscopy of Alkali Atoms (Li, Na, K) Attached to Highly Quantum Clusters. *J. Phys. Chem. A* **1998**, *102*, 95–101.
186. Schreiber, F.; Eberhardt, A.; Leung, T. Y. B.; Schwartz, P.; Wetterer, S. M.; Lavrich, D. J.; Berman, L.; Fenter, P.; Eisenberger, P.; Scoles, G. Adsorption Mechanisms, Structures and Growth Regimes of an Archetypal Self-Assembling System: Decanethiol on Au(111). *Phys. Rev. B: Condens. Matter Mater. Phys.* **1998**, *57* (19), 12476–12481.
187. Higgins, J.; Reho, J.; Callegari, C.; Ernst, W. E.; Stienkemeier, F.; Scoles, G. He Cluster-Isolation Spectroscopy: Alkali Dimers in the Triplet Manifold. *J. Phys. Chem. A* **1998**, *102*, 4952–4965.
188. Fenter, P.; Schreiber, F.; Berman, L.; Scoles, G.; Eisenberger, P.; Bedzyk, M. J. On the Structure and Evolution of the Buried S/Au Interface in Self-Assembled Monolayers: X-ray Standing Wave Results. *Surf. Sci.* **1998**, *412/413*, 213.
189. Schwartz, P.; Schreiber, F.; Eisenberger, P.; Scoles, G. Growth Kinetics of Decane Thiol Monolayers Self-Assembled on Au(111) by Molecular Beam Deposition: An Atomic Beam Diffraction Study. *Surf. Sci.* **1999**, *423*, 208–224.
190. Reinhard, I.; Callegari, C.; Conjusteau, A.; Lehmann, K. K.; Scoles, G. Single and Double Resonance Microwave Spectroscopy in Superfluid Helium Clusters. *Phys. Rev. Lett.* **1999**, *82*, 5036–5039.
191. Libuda, J.; Scoles, G. Collision Induced Chemical Dynamics in Ethanethiol Adsorbed on Au(111). *J. Phys. Chem. B* **1999**, *103* (45), 9933–9943.
192. Chizhov, I.; Kahn, A.; Scoles, G. Initial Growth of 3,4,9,10-Perylenetetracarboxylic-dianhydride (PTCDA) on Au(111): A Scanning Tunneling Microscopy Study. *J. Cryst. Growth* **1999**, *208*, 449–458.
193. Merker, U.; Srivastava, H. K.; Callegari, A.; Lehmann, K. K.; Scoles, G. Eigenstate Resolved Infrared and Millimeter-Wave-Infrared Double Resonance Spectroscopy of Methylamine in the N–H Stretch First Overtone Region. *Phys. Chem. Chem. Phys.* **1999**, *1*, 2427–2433.
194. Callegari, C.; Conjusteau, A.; Reinhard, I.; Lehmann, K. K.; Scoles, G. From Intermolecular Forces to Condensed Phase Spectroscopy: Ro-vibrational Spectroscopy Inside Superfluid Nanodroplets. In *Proceedings of the CCP6 Workshop on Rovibrational Bound States in Polyatomic Molecules*, University of Aberdeen, Scotland, April 11–14, 1999.
195. Callegari, C.; Conjusteau, A.; Reinhard, I.; Lehmann, K. K.; Scoles, G.; Dalfonso, F. A Superfluid Hydrodynamic Model for the Enhanced Moments of Inertia of Molecules in Liquid ^4He . *Phys. Rev. Lett.* **1999**, *83* (24), 5058–5061; **2000**, *84*, 1848.
196. Schreiber, F.; Gerstenberg, M. C.; Edinger, B.; Toperverg, B.; Forrest, S. R.; Scoles, G.; Dosch, H. Phase-Sensitive Surface X-ray Scattering Study of a Crystalline Organic–Organic Heterostructure. *Physica B* **2000**, *283*, 75–78 (6SXNS Proceedings).
197. Gerstenberg, M. C.; Schreiber, F.; Leung, T. Y. B.; Bracco, G.; Forrest, S. R.; Scoles, G. Organic Semiconducting Thin Film Growth on an Organic Substrate: 3,4,9,10-Perylenetetracarboxylicdianhydride (PTCDA) on a Monolayer of Decanethiol Self-Assembled on Au(111). *Phys. Rev. B: Condens. Matter Mater. Phys.* **2000**, *61* (11), 7678–7685.
198. Libuda, J.; Scoles, G. Collision Induced Desorption of Hydrocarbons Physisorbed on Au(111). *J. Chem. Phys.* **2000**, *112*, (3) 1522–1530.
199. Reho, J. H.; Merker, U.; Radcliff, M. R.; Lehmann, K. K.; Scoles, G. Spectroscopy and Dynamics of Al Atoms Solvated in Superfluid Helium Nanodroplets. *J. Phys. Chem. A* **2000**, *104*, 3620–3626.
200. Sin, J. M.; Nayak, S.; Scoles, G. On the Nature of Bonding in Small Mg Clusters. In *Cluster and Nanostructure Interfaces*; Jena, P., Khanna, S. N., Rao, B. K., Eds.; World Scientific: River Edge, NJ, 2000; p 345.
201. Chizhov, I.; Scoles, G.; Kahn, A. The Influence of Steps on the Orientation of Copper Phthalocyanine Monolayers on Au(111). *Langmuir* **2000**, *16*, 4358–4361.
202. Higgins, J.; Hollebeek, T.; Reho, J.; Ho, T. S.; Lehmann, K. K.; Rabitz, H.; Scoles, G.; Gutowski, M. On the Importance of Exchange Effects in Three-Body Interactions: The Lowest Quartet State of Na_3 . *J. Chem. Phys.* **2000**, *112* (13), 5751–5761.
203. Callegari, C.; Reinhard, I.; Lehmann, K. K.; Scoles, G.; Nauta, K.; Miller, R. E. Finite Size Effects and Rotational Relaxation in Superfluid Helium Nanodroplets: Microwave-Infrared Double-Resonance Spectroscopy of Cyanoacetylene. *J. Chem. Phys.* **2000**, *113*, 4636–4646.

204. Ho, T.-S.; Rabitz, H.; Scoles, G. Reproducing Kernel Technique for Extracting Accurate Potentials from Spectral Data: Potential Curves of the Two Lowest States $X^1\Sigma_g^+$ and a $^3\Sigma_u^+$ of the Sodium Dimer. *J. Chem. Phys.* **2000**, *112* (14), 6218–6227.
205. Reho, J.; Merker, U.; Radcliff, M. R.; Lehmann, K. K.; Scoles, G. Spectroscopy of Mg Atoms Solvated in Helium Nanodroplets. *J. Chem. Phys.* **2000** *112* (19), 8409–8416.
206. Leung, T. Y. B.; Schwartz, P.; Scoles, G.; Schreiber, F.; Ulman, A. Structure and Growth of 4-Methyl-4'-mercaptobiphenyl Monolayers on Au(111): A Surface Diffraction Study. *Surf. Sci.* **2000**, *458*, 34–52.
207. Conjusteau, A.; Callegari, C.; Reinhard, I.; Lehmann, K. K.; Scoles, G. Microwave Spectra of HCN and DCN in ^4He Nanodroplets: A Test of Adiabatic Following. *J. Chem. Phys.* **2000**, *113* (12), 4840–4843.
208. Callegari, C.; Conjusteau, A.; Reinhard, I.; Lehmann, K. K.; Scoles, G. First Overtone Helium Nanodroplet Isolation Spectroscopy of Molecules Bearing the Acetylenic CH Chromophore. *J. Chem. Phys.* **2000**, *113* (23) 10535–10550.
209. Leung, T. Y. B.; Gerstenberg, M. C.; Lavrich, D. J.; Scoles, G.; Schreiber, F.; Poirier, G. 1,6-Hexanedithiol Monolayers on Au(111): A Multitechnique Structural Study. *Langmuir* **2000**, *16*, 549–561.
210. Srivastava, H. K.; Conjusteau, A.; Mabuchi, H.; Callegari, A.; Lehmann, K. K.; Scoles, G. A Sub-Doppler Resolution Double Resonance Molecular Beam Infrared Spectrometer Operating at Chemically Relevant Energies (~ 2 eV). *Rev. Sci. Instrum.* **2000**, *71* (11), 4032–4038.
211. Srivastava, H. K.; Conjusteau, A.; Mabuchi, H.; Callegari, A.; Lehmann, K. K.; Scoles, G. Rovibrational Spectroscopy of the $v = 6$ Manifold in $^{12}\text{C}_2\text{H}_2$ and $^{13}\text{C}_2\text{H}_2$. *J. Chem. Phys.* **2000**, *113* (17), 7376–7383.
212. Callegari, A.; Merker, U.; Engels, P.; Srivastava, H. K.; Lehmann, K. K.; Scoles, G. Intramolecular Vibrational Redistribution in Aromatic Molecules I: Eigenstate Resolved CH Stretch First Overtone Spectra of Benzene. *J. Chem. Phys.* **2000**, *113* (23), 10583–10596.
213. Reho, J.; Higgins, J.; Callegari, C.; Lehmann, K. K.; Scoles, G. Alkali–Helium Exciplex Formation on the Surface of Helium Nano-Droplets. I. Dispersed Emission Spectroscopy. *J. Chem. Phys.* **2000**, *113* (21), 9686–9693.
214. Reho, J.; Higgins, J.; Lehmann, K. K.; Scoles, G. Alkali–Helium Exciplex Formation on the Surface of Helium Nanodroplets. II. A Time-Resolved Study. *J. Chem. Phys.* **2000**, *113*, 9694–9701.
215. Higgins, J.; Reho, J.; Stienkemeier, F.; Ernst, W. E.; Lehmann, K. K.; Scoles, G. Spectroscopy in, on and off a Beam of Superfluid Helium Nanodroplets. In *Atomic and Molecular Beams: The State of the Art 2000*; Campargue, R., Ed.; Springer: New York, 2000; Part VI, pp 723–754.
216. Vargas, M. C.; Giannozzi, P.; Selloni, A.; Scoles, G. Coverage-Dependent Adsorption of CH_3S and $(\text{CH}_3\text{S})_2$ on Au(111): A Density Functional Theory Study. *J. Phys. Chem. B* **2001**, *105*, 9509–9513.
217. Higgins, J.; Conjusteau, A.; Scoles, G.; Bernasek, S. L. State Selective Vibrational ($2\nu(3)$) Activation of the Chemisorption of Methane on Pt(111). *J. Chem. Phys.* **2001**, *114* (12), 5277–5283.
218. Wu, X.; Vargas, M. C.; Nayak, S.; Lotrich, V.; Scoles, G. Towards Extending the Applicability of Density Functional Theory to Weakly Bound Systems. *J. Chem. Phys.* **2001**, *115* (19), 8748–8757.
219. Callegari, C.; Lehmann, K. K.; Schmied, R.; Scoles, G. Helium Nanodroplet Isolation Ro-vibrational Spectroscopy: Methods and Recent Results. *J. Chem. Phys.* **2001**, *115* (22), 10090–10110.
220. Reho, J. H.; Higgins, J. H. P.; Nooijen, M.; Lehmann, K. K.; Scoles, G.; Gutowski, M. Photoinduced Nonadiabatic Dynamics in Quartet Na_3 and K_3 Formed Using Helium Nanodroplet Isolation. *J. Chem. Phys.* **2001**, *115* (22) 10265–10274.
221. Pflaum, J.; Bracco, G.; Schreiber, F.; Colorado, R., Jr.; Shmakora, O. E.; Lee, T. R.; Scoles, G.; Kahn, A. Structure and Electronic Properties of CH_3 - and CF_3 -Terminated Alkanethiol Monolayers on Au(111): A Scanning Tunneling Microscopy, Surface X-ray and Helium Scattering Study. *Surf. Sci.* **2002**, *498*, 89–104.
222. Bracco, G.; Acker, J.; Ward, M. D.; Scoles, G. He Diffraction Study of Organic Single Crystal Surfaces: Hydrogen-Bonded and Methyl-Terminated (001) Cleavage Planes of a Guanidinium Methanesulfonate Crystal. *Langmuir* **2002**, *18* (14), 5551–5557.
223. Danisman, M.; Casalis, L.; Bracco, G.; Scoles, G. Structural Investigation of Monolayers Prepared by Deposition of $(\text{CH}_3\text{S})_2$ on the (111) Face of Single-Crystal Gold. *J. Phys. Chem. B* **2002**, *106*, 11771–11777.
224. Callegari, C.; Pearman, R.; Choi, S.; Engels, P.; Srivastava, H.; Gruebele, M.; Lehmann, K. K.; Scoles, G. Intramolecular Vibrational Relaxation in Aromatic Molecules II: An Experimental and Computational Study of Pyrrole and Triazine near the IVR Threshold. *Mol. Phys.* **2003**, *101* (4–5), 551–568.
225. Giannozzi, P.; Car, R.; Scoles, G. Oxygen Adsorption on Graphite and Nanotubes. *J. Chem. Phys.* **2003**, *118* (3), 1003–1006.
226. Case, M.; McLendon, G.; Hu, Y.; Vanderlick, T. K.; Scoles, G. Using Nanografting to Achieve Directed Assembly of de novo Designed Metalloproteins on Gold. *Nano Lett.* **2003**, *3* (4), 425–429.
227. Schwartz, P. V.; Lavrich, D. J.; Scoles, G. Overlays of Long-Chain Organic Molecules Physisorbed on the Surface of Self-Assembled Monolayers of Alkylthiols on Au(111). *Langmuir* **2003**, *19*, 4969–4976.
228. Ruiz, R.; Nickel, B.; Koch, N.; Feldman, L. C.; Haglund, R.; Kahn, A.; Scoles, G. Pentacene Ultrathin Film Formation on Reduced and Oxidized Si Surfaces. *Phys. Rev. B: Condens. Matter Mater. Phys.* **2003**, *67*, 125406.
229. Casalis, L.; Danisman, M. F.; Nickel, B.; Bracco, G.; Toccoli, T.; Iannotta, S.; Scoles, G. Hyperthermal Molecular Beam Deposition of Highly Ordered Organic Thin Films. *Phys. Rev. Lett.* **2003**, *90* (20), 206101.
230. Bracco, G.; Ward, M. D.; Scoles, G. Atomic Diffraction Study of the Interaction of He Atoms with the Surface of an Organic Single Crystal: The (001) Cleavage Planes of Guanidinium Methanesulfonate. *J. Chem. Phys.* **2003**, *118*, 8405–8410.
231. Bracco, G.; Scoles, G. Study of the Interaction Potential between a He Atom and a SAM of Decanethiol. *J. Chem. Phys.* **2003**, *119*, 6277.

232. Bracco, G.; Hu, Y.; Acker, J.; Ward, M. D.; Scoles, G.; Study of the (001) Cleavage Planes of Guanidinium Methanesulfonate Single Crystals by AFM and He Diffraction. *Appl. Surf. Sci.* **2003**, *151*, 212–213.
233. Schreiber, F.; Gerstenberg, M. G.; Dosch, H.; Scoles, G. Melting Point Enhancement of a SAM Induced by a van der Waals Bound Capping Layer. *Langmuir* **2003**, *19*, 10004–10006.
234. Piccinin, S.; Selloni, A.; Scandolo, S.; Car, R.; Scoles, G. Electronic Properties of Metal–Molecule–Metal Systems at Zero Bias: A Periodic Density Functional Study. *J. Chem. Phys.* **2003**, *119*, 6729–6781.
235. Ruiz, R.; Nickel, B.; Koch, N.; Feldman, L. C.; Haglund, R. F., Jr.; Kahn, A.; Family, F.; Scoles, G. Dynamic Scaling, Island Size Distribution and Morphology in the Aggregation Regime of Sub-monolayer Pentacene Films. *Phys. Rev. Lett.* **2003**, *91*, 136102.
236. Çarçabal, P.; Schmied, R.; Lehmann, K. K.; Scoles, G. Helium Nano Droplet Isolation Spectroscopy of Perylene and its Complexes with Oxygen. *J. Chem. Phys.* **2004**, *120* (14), 6792–6793.
237. Suo, Z.; Gao, Y. F.; Scoles, G. Nanoscale Domain Stability in Organic Monolayers on Metals. *J. Appl. Mech.* **2004**, *71*, 24–31.
238. Schmied, R.; Carcabal, P.; Dokter, A. M.; Lonij, V. P. A.; Lehmann, K. K.; Scoles, G. UV Spectra of Benzene Isotopomers and Dimers in Helium Nanodroplets. *J. Chem. Phys.* **2004**, *121* (6), 2701–2710.
239. Nickel, B.; Barabash, R.; Ruiz, R.; Koch, N.; Kahn, A.; Feldman, L. C.; Haglund, R. F.; Scoles, G. Dislocation Arrangements in Pentacene Thin Films. *Phys. Rev. B: Condens. Matter Mater. Phys.* **2004**, *70*, 125401.
240. Ruiz, R.; Mayer, A. C.; Malliaras, G. G.; Nickel, B.; Scoles, G.; Kazimirov, A.; Kim, H.; Headrick, R. L.; Islam, Z. Structure of Pentacene Thin Films. *Appl. Phys. Lett.* **2004**, *85* (21), 4926–4928.
241. Scheele, I.; Conjusteau, A.; Callegari, C.; Schmied, R.; Lehmann, K. K.; Scoles, G. Near-Infrared Spectroscopy of Ethylene and Ethylene Dimer in Superfluid Helium Droplets. *J. Chem. Phys.* **2005**, *122* (10), 104307.
242. Houston, J. E.; Doelling, C. M.; Vanderlick, T. K.; Hu, Y.; Scoles, G.; Wenzl, I.; Lee, T. R. Comparative Study of the Adhesion, Friction, and Mechanical Properties of CF_3 - and CH_3 -Terminated Alkanethiol Monolayers. *Langmuir* **2005**, *21* (9), 3926–3932.
243. Danisman, M. F.; Casalis, L.; Scoles, G. Supersonic Molecular Beam Deposition of Pentacene Thin Films on Two Ag(111) Surfaces with Different Step Densities. *Phys. Rev. B: Condens. Matter Mater. Phys.* **2005**, *72* (8), 085404.
244. Sun, Q.; Selloni, A.; Scoles, G. Electron Tunneling through Molecular Media: A Density Functional Study of Au/Dithiol/Au Systems. *ChemPhysChem* **2005**, *6* (9), 1906–1910.
245. Hu, Y.; Das, A.; Hecht, M. H.; Scoles, G. Nanografting De Novo Proteins onto Gold Surfaces. *Langmuir* **2005**, *21* (20), 9103–9109.
246. Liang, J.; Sun, Q.; Selloni, A.; Scoles, G. Side-by-Side Characterization of Electron Tunneling through Monolayers of Isomeric Molecules: A Combined Experimental and Theoretical Study. *J. Phys. Chem. B* **2006**, *110*, 24797–24801.
247. Lazzarino, M.; De Marchi, E.; Bressanutti, M.; Vaccari, L.; Cabrini, S.; Schmid, C.; Poetes, R.; Scoles, G. Twin Cantilevers with a Nanogap for Single Molecule Experimentation. *Microelectron. Eng.* **2006**, *83*, 1309–1311.
248. Sun, Q.; Selloni, A.; Scoles, G. Electronic Structure of Metal/Molecule/Metal Junctions: A Density Functional Theory Study of the Influence of the Molecular Terminal Group. *J. Phys. Chem. B* **2006**, *110* (8), 3493–3498.
249. Mazzarello, R.; Cossaro, A.; Verdini, A.; Rousseau, R.; Casalis, L.; Danisman, M. F.; Floreano, L.; Scandolo, S.; Morgante, A.; Scoles, G. Structure of a CH_3S Monolayer on Au(111) Solved by the Interplay between Molecular Dynamics Calculations and Diffraction Measurements. *Phys. Rev. Lett.* **2007**, *98* (1), 016102.
250. Castronovo, M.; Bano, F.; Raugei, S.; Scaini, D.; Dell'Angela, M.; Hudej, R.; Casalis, L.; Scoles, G. Mechanical Stabilization Effect of Water on a Membrane-like System. *J. Am. Chem. Soc.* **2007**, *129* (9), 2636–2641.
251. Qazi, A.; Nonis, D.; Pozzato, A.; Tormen, M.; Lazzarino, M.; Carrato, S.; Scoles, G. Asymmetrical Twin Cantilevers for Single Molecule Detection. *Appl. Phys. Lett.* **2007**, *90* (17), 173118.
252. Liang, J.; Scoles, G. Nanografting of Alkanethiols by Tapping Mode Atomic Force Microscopy. *Langmuir* **2007**, *23* (11), 6142–6147.
253. Birer, O.; Moreschini, P.; Lehmann, K. K.; Scoles, G. Electronic Spectroscopy of Nonalternant Hydrocarbons inside Helium Nanodroplets. *J. Phys. Chem. A* **2007**, *111*, 12200.