

## Publications of Michael L. Klein

## Books

1. *Rare Gas Solids*; Klein, M. L., Venables, J. A., Eds.; Academic Press: London, 1976; Vol. I, pp 1–608.
2. *Rare Gas Solids*; Klein, M. L., Venables, J. A., Eds.; Academic Press: London, 1977; Vol. II, pp 609–1252.
3. *Inert Gases*; Klein, M. L., Ed.; Springer Series in Chemical Physics 34; Springer: New York, 1984.

## Articles and Chapters

4. Barron, T. H. K.; Klein, M. L. Thermal and elastic properties of crystals at low temperatures. *Phys. Rev.* **1962**, *127*, 1997–1998.
5. Barron, T. H. K.; Klein, M. L. Lattice dynamic of anharmonic crystals near  $T = 0$ . In *Proceedings of the Eighth International Conference on Low Temperature Physics*; Butterworth: London, 1962; 415–416.
6. Barron, T. H. K.; Klein, M. L. On the strain dependence of the vibrational frequency distributions of simple lattices. *Proc. Phys. Soc.* **1963**, *82*, 161–173.
7. Klein, M. L. Anharmonic forces and the vapor pressure ratio of monatomic isotopic solids. *J. Chem. Phys.* **1964**, *41*, 749–755.
8. Klein, M. L.; Reissland, J. A. Anharmonic forces and the vapor pressure ratio of monatomic isotopic solids II. *J. Chem. Phys.* **1964**, *41*, 2778–2776.
9. Johnson, J. D.; Klein, M. L. Forces between adsorbed atoms and the determination of surface areas of solids. *Trans. Faraday Soc.* **1964**, *60*, 1964–1972.
10. Barron, T. H. K.; Klein, M. L. Second-order elastic constants of a solid under stress. *Proc. Phys. Soc.* **1964**, *85*, 523–532.
11. Everett, D. H.; Johnson, J. D.; Klein, M. L. High temperature adsorption and interactions between adsorbed atoms. In *An. R. Soc. Esp. Fis. Quim., Ser. A* **1965**, *61*, 73–92.
12. Casanova, G.; de Paz, M.; Dondi, M. G.; Klein, M. L.; Scoles, G. Isotope effects in physical adsorption. *Discuss. Faraday Soc.* **1965**, *40*, 188–193.
13. Barron, T. H. K.; Klein, M. L. Thermoelastic properties of some cubic close packed lattices. *Proc. Phys. Soc.* **1965**, *85*, 533–558.
14. Klein, M. L. Quantum second virial coefficient of a Lennard-Jones gas. *Mol. Phys.* **1965**, *10*, 87–89.
15. Feldman, C.; Feldman, J. L.; Horton, G. K.; Klein, M. L. Anharmonic contributions in the gruneisen parameters of solid argon, krypton and xenon. *Proc. Phys. Soc.* **1967**, *90*, 1182–1185.
16. Johnson, J. D.; Klein, M. L. Interactions between physically adsorbed molecules. *J. Chem. Phys.* **1967**, *47*, 1035–1037.
17. Klein, M. L.; Munn, R. J. Interaction potential of the inert gases. *J. Chem. Phys.* **1967**, *47*, 1035–1037.
18. Feldman, C.; Klein, M. L. On the velocity of sound in solid argon. *Phys. Lett. A* **1967**, *25*, 190–191.
19. de Paz, M.; Turi, B.; Klein, M. L. New self diffusion measurements in Ar gas. *Physica* **1967**, *36*, 127–135.
20. Segal, G. A.; Klein, M. L. Calculations of infrared intensities by the CNDO method. *J. Chem. Phys.* **1967**, *47*, 4236–4240.
21. Casanova, G.; Dondi, M. G.; Scoles, G.; Klein, M. L. Isotope separation factor in physical adsorption and the interaction between argon atoms and graphitized carbon blacks. In *Fundamentals of Gas Surface Interactions*; Academic Press: New York, 1967; pp 258–270.
22. Klein, M. L.; Horton, G. K. Thermodynamic properties of rare gas solids Ar, Kr and Xe. In *Proceedings of LT II*, St. Andrews, U. K., 1968; Vol. 1, pp 553–567.
23. Feldman, C.; Klein, M. L. On the elastic constants of polycrystalline argon. *Philos. Mag.* **1968**, *17*, 135–140.
24. Goldman, V. V.; Horton, G. K.; Klein, M. L. An improved self consistent phonon approximation. *Phys. Rev. Lett.* **1968**, *21*, 1527–1529.
25. Goldman, V. V.; Horton, G. K.; Klein, M. L. An improved self-consistent phonon theory for neon. *Phys. Lett. A* **1968**, *28*, 341–342.
26. Klein, M. L. On the second order elastic constants of molecular solids. In *Proceedings of the Second Materials Research Symposium*; NBS Special Publication 301; U.S. Government Printing Office: Washington, DC, 1969; pp 349–351.
27. Klein, M. L.; Morrison, J. A.; Weir, R. D. Molecular motions in solid isotopic silanes. *Discuss. Faraday Soc.* **1969**, *48*, 93–101.
28. Klein, M. L.; Goldman, V. V.; Horton, G. K. On the temperature dependence of the cubic anharmonic contribution to the Helmholtz free energy of a simple crystal model. *J. Phys. C: Solid State Phys.* **1969**, *2*, 1542–1549.
29. Klein, M. L.; Horton, G. K.; Feldman, J. L. Thermodynamics properties of solid Ar, Kr and Xe based upon a short-range central force and the conventional perturbation expansion of the partition function. *Phys. Rev.* **1969**, *184*, 968–978.
30. Feldman, C.; Klein, M. L.; Horton, G. K. Calculation of the temperature dependence of the second-order elastic constants of fcc, Ar, Kr and Xe using a two-body short-range interatomic potential. *Phys. Rev.* **1969**, *184*, 910–918.
31. Goldman, V. V.; Horton, G. K.; Klein, M. L. A theoretical study of the lattice dynamics of neon and its isotopes. *J. Low Temp. Phys.* **1969**, *1*, 391–405.
32. Chell, G. G.; Goldman, V. V.; Klein, M. L.; Horton, G. K. Lattice dynamics of  $^3\text{He}$  and  $^4\text{He}$  at high pressures. *Phys. Rev. B* **1970**, *2*, 560–561.
33. Klein, M. L.; Blizard, W.; Goldman, V. V. Calculation of the vapor–pressure ratio of the isotopes of solid Ne and Ar. *J. Chem. Phys.* **1970**, *52*, 1633–1635.
34. Goldman, V. V.; Horton, G. K.; Klein, M. L. Phonon energies and lifetimes in solid Ne and He in the first-order self-consistent approximation. *Phys. Rev. Lett.* **1970**, *24*, 1424–1427.
35. Klein, M. L.; Chell, G. G.; Goldman, V. V.; Horton, G. K. Volume dependence of self-consistent phonon energies. *J. Phys. C: Solid State Phys.* **1970**, *3*, 806–809.

36. Klein, M. L.; Goldman, V. V.; Horton, G. K. Thermodynamic properties of solid Ar, Kr and Xe based upon a short-range central force and the improved self-consistent phonon scheme. *J. Phys. Chem. Solids* **1970**, *31*, 2441–2452.
37. Barker, J. A.; Klein, M. L.; Bobetic, M. V. Elastic constants and phonon dispersion curves for solid argon near 0 °K. *Phys. Rev. B* **1970**, *2*, 4176–4179.
38. Klein, M. L.; Koehler, T. R. Lattice dynamics of hcp ortho-deuterium. *Phys. Lett. A* **1970**, *33*, 253–254.
39. Klein, M. L.; Koehler, T. R. Self-consistent phonon spectrum of hcp H<sub>2</sub> and D<sub>2</sub>. *J. Phys. C: Solid State Phys.* **1970**, *3*, L102–104.
40. Klein, M. L.; Horton, G. K.; Goldman, V. V. Self-consistent theory of second-order elastic constants with an application to the noble-gas crystals. *Phys. Rev. B* **1970**, *2*, 4995–5002.
41. Horton, G. K.; Goldman, V. V.; Klein, M. L. Neutron and Brillouin scattering in quantum crystals. *J. Appl. Phys.* **1970**, *41*, 5138–5140.
42. Goldman, V. V.; Horton, G. K.; Keil, T. H.; Klein, M. L. Phonon energies and lifetimes in solid argon near 0 °K. *J. Phys. C: Solid State Phys.* **1970**, *3*, L33–36.
43. Glyde, H. R.; Klein, M. L. Anharmonic effects and the lattice dynamics of insulators. *CRC Crit. Rev. Solid State Sci.* **1971**, *2*, 181–254.
44. Klein, M. L.; Hoover, W. G. Comparison of classical Monte Carlo experiments with self-consistent phonon theory: Elastic constants for solid xenon. *Phys. Rev. B* **1971**, *4*, 537–538.
45. Klein, M. L.; Hoover, W. G. Comparison of classical Monte Carlo experiments with improved self-consistent phonon theory: Thermodynamic properties of solid Xe. *Phys. Rev. B* **1971**, 539–542.
46. Barker, J. A.; Klein, M. L.; Bobetic, M. V.; Zucker, I. J. Three-body interactions and lattice sums in crystals. *J. Phys. C: Solid State Phys.* **1971**, *4*, L355–357.
47. Klein, M. L.; Barker, J. A.; Koehler, T. R. Lattice dynamics of FCC argon with three-body forces. *Phys. Rev. B* **1971**, *4*, 1983–1990.
48. Goldman, V. V.; Horton, G. K.; Klein, M. L. Relationship between adiabatic elastic constants and the slopes of phonon dispersion curves for rare-gas solids. *Phys. Rev. B* **1971**, *4*, 567.
49. Barker, J. A.; Bobetic, M. V.; Klein, M. L. Lattice dynamics of solid Kr. *Phys. Lett. A* **1971**, *24*, 415–416.
50. Barker, J. A.; Klein, M. L. Scattering measurements, second virial coefficients and the interatomic potential for argon. *Chem. Phys. Lett.* **1971**, *11*, 501–503.
51. Bobetic, M. V.; Barker, J. A.; Klein, M. L. Lattice dynamics with three-body forces. II. Krypton. *Phys. Rev. B* **1972**, *5*, 3185–3189.
52. Klein, M. L.; Martin, D. L. Comments on the claimed difference between the thermal and elastic Debye temperatures of copper near 0° K. *Phys. Lett. A* **1972**, *38*, 430.
53. Klein, M. L.; Murphy, R. D. Elastic constants of solid Ar, Kr and Xe: A Monte Carlo study. *Phys. Rev. B* **1972**, *6*, 2433–2442.
54. Klein, M. L.; Horton, G. K. The rise of self-consistent phonon theory. *J. Low Temp. Physics* **1972**, *9*, 151–166.
55. Klein, M. L. Monte Carlo study of the elastic constants of compressed argon. *Chem. Phys. Lett.* **1973**, *18*, 203–204.
56. Klein, M. L.; Koehler, T. R.; Gray, R. L. Thermodynamic properties of solid argon and krypton. *Phys. Rev. B* **1973**, *7*, 4707–4712.
57. Barker, J. A.; Klein, M. L. Monte Carlo calculations for solid and liquid argon. *Phys. Rev. B* **1973**, *7*, 4707–4712.
58. Klein, M. L. Comments on the interatomic potential of Ne. *Chem. Phys. Lett.* **1973**, *18*, 203–204.
59. Gibbons, T. G.; Klein, M. L.; Murphy, R. D. The elastic constants of solid Ar. *Chem. Phys. Lett.* **1973**, *18*, 325–328.
60. Farrar, J. M.; Lee, Y. T.; Goldman, V. V.; Klein, M. L. Neon interatomic potentials from scattering data and crystalline properties. *Chem. Phys. Lett.* **1973**, *19*, 359–362.
61. Goldman, V. V.; Klein, M. L. An interatomic potential for Ne<sub>2</sub> derived from solid-state data. *J. Low Temp. Phys.* **1973**, *12*, 101–103.
62. Buck, U.; Dondi, M. G.; Valbusa, U.; Klein, M. L.; Scoles, G. Determination of the interatomic potential for krypton. *Phys. Rev. A* **1973**, *8*, 2409–2416.
63. Murphy, R. D.; Klein, M. L. Radial distribution function of liquid sodium. *Phys. Rev. A* **1973**, *8*, 2640–26–44.
64. Barron, T. H. K.; Klein, M. L. Perturbation theory of anharmonic crystals. In *Lattice Dynamics*; Horton, G. K., Maradudin, A. A., Eds.; North-Holland: Amsterdam, 1974; pp 391–449.
65. Hansen, J. P.; Klein, M. L. Computer ‘experiments’ on solid rare gases: The dynamical structure factor  $S(\mathbf{Q}, \omega)$ . *J. Phys.* **1974**, *35*, L29–L31.
66. Gibbons, T. G.; Klein, M. L. Thermodynamic properties for a simple model of solid carbon dioxide, Monte Carlo, cell model and quasi-harmonic calculations. *J. Chem. Phys.* **1974**, *60*, 112–126.
67. Cohen, S. S.; Klein, M. L. Interatomic potentials and phonon spectra of dilute rare-gas mixtures. *J. Chem. Phys.* **1974**, *61*, 3210–3216.
68. Gibbons, T. G.; Klein, M. L. A Monte Carlo computer simulation of the thermodynamic properties of solid N<sub>2</sub>. *Chem. Phys. Lett.* **1974**, *29*, 463–465.
69. Le Roy, R. J.; Klein, M. L.; McGee, I. J. On the dissociation energy and interaction potential of ground-state Ne<sub>2</sub>. *Mol. Phys.* **1974**, *28*, 587–591.
70. Jacucci, G.; Klein, M. L.; McDonald, I. R. A molecular dynamics study of the lattice vibrations of sodium chloride. *J. Phys.* **1975**, *36*, L97–L100.
71. Cohen, S. S.; Klein, M. L. Thermodynamic properties of potassium at 160 and 308 K. *Phys. Rev. B* **1975**, *12*, 2984–2987.
72. Goldman, V. V.; Klein, M. L. Difference between zero- and first-sound propagation in solid Kr. *Phys. Rev. B* **1975**, *12*, 4577–4580.
73. Weis, J. J.; Klein, M. L. The dynamical structure factor  $S(\mathbf{Q}, \omega)$  of solid  $\alpha$ -N<sub>2</sub>. *J. Chem. Phys.* **1975**, *63*, 2869–2873.
74. Hansen, J. P.; Klein, M. L. Dynamical structure factor  $S(\mathbf{Q}, \omega)$  of rare-gas solids. *Phys. Rev. B* **1976**, *13*, 878–887.

75. Cohen, S. S.; Klein, M. L.; Duesbery, M. S.; Taylor, R. Computer simulation of bulk properties of alkali metals. In *Proceedings of the International Conference on Computer Simulation for Materials Applications*; American Institute of Metallurgical Engineers: New York, 1976; pp 619–628.
76. Klein, M. L.; Koehler, T. R. Lattice dynamics of rare gas solids. In *Rare Gas Solids*; Klein, M. L., Venables, J. A., Eds.; Academic Press: London, 1976; pp 326–381.
77. Cohen, S. S.; Klein, M. L.; Duesbery, M. S.; Taylor, R. A computer simulation of thermodynamic properties of solid Na. *J. Phys. F: Met. Phys.* **1976**, *6*, 337–347.
78. Barker, J. A.; Klein, M. L.; Bobetic, M. V. Lattice dynamics with 3-body forces III. Solid Xe and Kr. *IBM J. Res. Dev.* **1976**, *20*, 222–227.
79. Goldman, V. V.; Klein, M. L. Lattice dynamics of solid Ne. *J. Low Temp. Phys.* **1976**, *22*, 501–506.
80. McDonald, I. R.; Klein, M. L. Simulation of liquid ammonia. *J. Chem. Phys.* **1976**, *64*, 4790–4791.
81. Goldman, V. V.; Klein, M. L. Self-consistent phonon calculation of the elastic constants of the  $\beta$ -phase of solid  $N_2$ . *J. Chem. Phys.* **1976**, *64*, 5121–5125.
82. Cowley, E. R.; Jacucci, G.; Klein, M. L.; McDonald, I. R. Anharmonic effects in the phonon spectra of sodium chloride. *Phys. Rev. B* **1976**, *14*, 1758–1769.
83. Jacucci, G.; Klein, M. L.; Taylor, R. The static structure factor of liquid Li. *Solid State Commun.* **1976**, *19*, 657–659.
84. Cohen, S. S.; Klein, M. L.; Duesbury, M. S.; Taylor, R. Correction to a previous pseudopotential calculation of the elastic constants of sodium. *J. Phys. F: Met. Phys.* **1976**, *6*, L271–L273.
85. Alder, B. J.; Strauss, H. L.; Weis, J. J.; Hansen, J. P.; Klein, M. L. A molecular dynamics study of the intensity and band shapes of depolarized light scattered from rare gas crystals. *Physica B* **1976**, *83*, 249–258.
86. Hansen, J. P.; Klein, M. L. Dynamical structure factor  $S(Q, \omega)$  of solid potassium. *Solid State Commun.* **1976**, *20*, 771–773.
87. Klein, M. L.; O'Shea, S. F. Monte Carlo calculations of the elastic constants of xenon. *Chem. Phys. Lett.* **1977**, *48*, 555–559.
88. Klein, M. L.; Weis, J. J. The dynamical structure factor  $S(Q, \omega)$  of solid  $\beta$ - $N_2$ . *J. Chem. Phys.* **1977**, *67*, 217–224.
89. Jacucci, G.; Klein, M. L.; Taylor, R. Localized modes in Rb–K alloys. *Solid State Commun.* **1977**, *24*, 685–686.
90. Klein, M. L.; Jacucci, G. Anharmonic lattice dynamics of solid Al. *Phys. Rev. B* **1977**, *6*, 1322–1324.
91. Cohen, S. S.; Klein, M. L. Hydrogen atoms in solid Ar. *J. Chem. Phys.* **1977**, *67*, 2396.
92. Glyde, H. R.; Hansen, J. P.; Klein, M. L. Anharmonic lattice dynamics of solid potassium. *Phys. Rev. B* **1977**, *16*, 3476–3483.
93. Duquette, G.; Ellis, T. H.; Scoles, G.; Watts, R. O.; Klein, M. L. An intermolecular potential for  $(NH_3)_2$ . *J. Chem. Phys.* **1978**, *68*, 2544–2549.
94. Righini, R.; Klein, M. L. Lattice dynamics of solid ammonia. *J. Chem. Phys.* **1978**, *68*, 5553–5557.
95. McDonald, I. R.; Klein, M. L. Intermolecular potentials and the simulation of liquid water. *J. Chem. Phys.* **1978**, *68*, 4876–4877.
96. Klein, M. L.; McDonald, I. R.; O'Shea, S. F. An intermolecular force model for  $(HF)_2$ . *J. Chem. Phys.* **1978**, *69*, 63–66.
97. Jacucci, G.; Klein, M. L.; Taylor, R. Lattice dynamics of  $Rb_{71}K_{29}$ : A molecular dynamics study. *Phys. Rev. B* **1978**, *18*, 3782–3789.
98. Klein, M. L. Computer simulation of collective modes in solids. In *Computer Modeling of Matter*; Lykos, P., Ed.; ACS Symposium Series 86; American Chemical Society: Washington, DC, 1978; pp 94–110.
99. McDonald, I. R.; Klein, M. L. Molecular dynamics studies of hydrogen-bonded liquids. *Faraday Discuss. Chem. Soc.* **1978**, *66*, 48–57.
100. Sears, W. M.; Klein, M. L.; Morrison, J. A. Polyttypism and the vibrational properties of  $PbI_2$ . *Phys. Rev. B* **1979**, *19*, 2305–2313.
101. O'Shea, S. F.; Klein, M. L. Orientational phases of classical octupoles on a triangular lattice and the adsorption of methane on graphite. *J. Chem. Phys.* **1979**, *71*, 2398–2403.
102. Klein, M. L.; McDonald, I. R. Structure and dynamics of associated molecular systems. I. Computer simulation of liquid hydrogen fluoride. *J. Chem. Phys.* **1979**, *71*, 298–308.
103. Kobashi, K.; Klein, M. L.; Chandrasekharan, V. Lattice dynamics of solid oxygen. *J. Chem. Phys.* **1979**, *71*, 843–849.
104. Klein, M. L.; McDonald, I. R.; Righini, R. Structure and dynamics of associated molecular systems. II. Atom–atom potentials and the properties of ammonia. *J. Chem. Phys.* **1979**, *71*, 3673–3682.
105. Klein, M. L.; McDonald, I. R.; Berne, B. J.; Rao, M.; Beveridge, D. L.; Mehrotra, P. K. Radial correlations in associated liquids. *J. Chem. Phys.* **1979**, *71*, 3889–3891.
106. Buyers, W. J. L.; Dolling, G.; Klein, M. L.; Glyde, H. R. Anharmonic phonon response in aluminum: A neutron scattering test of computer simulation calculations. *Phys. Rev. B* **1979**, *20*, 4859–4863.
107. O'Shea, S. F.; Klein, M. L. Orientational phases of classical quadrupoles on a triangular net. *Chem. Phys. Lett.* **1979**, *66*, 381–383.
108. Jacucci, G.; Klein, M. L. Dynamical structure factor of metallic sodium at high temperatures. *Solid State Commun.* **1979**, *32*, 437–440.
109. Jacucci, G.; Klein, M. L. Structure and dynamics of metals at high temperatures. In *Liquid and Amorphous Metals*; Luscher, E., Coufal, H., Eds.; NATO ASI Series, Series E, Applied Sciences 36; Sijthoff & Noordhoff: Germantown, MD, 1980.
110. O'Shea, S. F.; Klein, M. L. Orientational ordering of quadrupoles on a simple cubic lattice. *Solid State Commun.* **1980**, *33*, 179–181.
111. Bounds, D. G.; Klein, M. L.; Patey, G. N. Molecular dynamics simulation of the plastic phase of solid methane. *J. Chem. Phys.* **1980**, *72*, 5348–5356.
112. McDonald, I. R.; O'Shea, S. F.; Bounds, D. G.; Klein, M. L. Structure and dynamics of associated molecular systems III: Computer simulation of liquid hydrogen chloride. *J. Chem. Phys.* **1980**, *72*, 5710–5717.
113. McDonald, I. R.; Bounds, D. G.; Klein, M. L. Structure and dynamics of associated molecular systems IV: The orientationally disordered phase I of solid DCl. *J. Chem. Phys.* **1980**, *73*, 532–537.



114. Klein, M. L.; Levesque, D.; Weis, J.-J. Molecular dynamics study of solid  $\gamma$ -O<sub>2</sub>. *Phys. Rev. B* **1980**, *21*, 5785–5792.
115. Kobashi, M.; Klein, M. L. Lattice vibrations of solid  $\alpha$ -F<sub>2</sub>. *Mol. Phys.* **1980**, *41*, 679–688.
116. Murthy, C. S.; Singer, K.; Klein, M. L.; McDonald, I. R. Effect of changes in pair potential on the dynamical structure factor of molecular crystals. *Mol. Phys.* **1980**, *40*, 1517–1521.
117. Patey, G. N.; Klein, M. L.; McDonald, I. R. Models for strongly polar liquids: The influence of molecular polarizability. *Chem. Phys. Lett.* **1980**, *73*, 375–378.
118. Murthy, C. S.; Singer, K.; Klein, M. L.; McDonald, I. R. Pairwise additive effective potentials for nitrogen. *Mol. Phys.* **1980**, *41*, 1387–1399.
119. Impey, R. W.; Klein, M. L.; McDonald, I. R. Molecular dynamics studies of the structure of water at high temperatures and density. *J. Chem. Phys.* **1981**, *74*, 647–652.
120. Hinchliffe, A.; Bounds, D. G.; Klein, M. L.; McDonald, I. R.; Righini, R. Intermolecular potentials for ammonia based in SCF-MO calculations. *J. Chem. Phys.* **1981**, *74*, 1211–1216.
121. Maki, K.; Klein, M. L. Phonon spectra of methane physisorbed on graphite. *J. Chem. Phys.* **1981**, *74*, 1488–1494.
122. Klein, M. L.; McDonald, I. R. Is hydrogen chloride an associated liquid? *Mol. Phys.* **1981**, *42*, 243–247.
123. Klein, M. L.; Levesque, D.; Weis, J.-J. Molecular dynamics study of solid nitrogen at high pressure. *Can. J. Phys.* **1981**, *59*, 539–534.
124. Klein, M. L.; Levesque, D.; Weis, J.-J. Molecular dynamics study of solid  $\beta$ -N<sub>2</sub>. *J. Chem. Phys.* **1981**, *74*, 2566–2568.
125. Klein, M. L.; McDonald, I. R. Comment on the structure of liquid ammonia. *J. Chem. Phys.* **1981**, *74*, 4214–4215.
126. Klein, M. L.; McDonald, I. R. Coupling of rotations and translations in cyanide crystals. *Chem. Phys. Lett.* **1981**, *78*, 383–387.
127. Righini, R.; Maki, K.; Klein, M. L. An intermolecular potential for methane. *Chem. Phys. Lett.* **1981**, *80*, 301–305.
128. Klein, M. L.; Goddard, J.; Bounds, D. G. An ab initio molecular orbital study of NaCN and KCN. *J. Chem. Phys.* **1981**, *75*, 3909–3915.
129. Klein, M. L.; McDonald, I. R. Molecular dynamics calculations for solid and liquid acetylene. *Chem. Phys. Lett.* **1981**, *80*, 76–81.
130. Bounds, D. G.; Klein, M. L.; McDonald, I. R. Anisotropy of the electrostatic interactions and the properties of orientationally disordered cyanide crystals. *Phys. Rev. Lett.* **1981**, *46*, 1682–1685.
131. Bounds, D. G.; Klein, M. L.; McDonald, I. R. Molecular dynamics study of phase I of RbCN. *Phys. Rev. B* **1981**, *24*, 3568–3570.
132. McDonald, I. R.; Bounds, D. G.; Klein, M. L. Molecular dynamics calculations for the liquid and cubic plastic crystal phases of carbon tetrachloride. *Mol. Phys.* **1982**, *45*, 521–542.
133. Reimer, J. R.; Watts, R. O.; Klein, M. L. Intermolecular potential functions and the properties of water. *Chem. Phys.* **1982**, *64*, 95–114.
134. Klein, M. L.; McDonald, I. R.; Ozaki, Y. Critical fluctuations in the paraelectric phase of NaNO<sub>2</sub>. *Phys. Rev. Lett.* **1982**, *48*, 1197–1200.
135. Righini, R.; Klein, M. L. Lattice dynamics of the high pressure monoclinic phase of solid carbon tetrachloride. *Chem. Phys. Lett.* **1982**, *87*, 604–606.
136. O'Shea, S. F.; Klein, M. L. Orientational phases of quadrupolar bilayers. *Phys. Rev. B* **1982**, *25*, 5882–5888.
137. Nosé, S.; Klein, M. L. Molecular dynamics study of solid argon with N<sub>2</sub>, O<sub>2</sub>, CO impurities. *Can. J. Phys.* **1982**, *60*, 1365–1370.
138. Klein, M. L.; McDonald, I. R.; Ozaki, Y. The rotor phase of solid caesium cyanide. *J. Phys. C: Solid State Phys.* **1982**, *15*, 4993–5002.
139. Klein, M. L.; McDonald, I. R. Properties of the paraelectric solid and molten phases of sodium nitrite. *Proc. R. Soc. London, Ser. A* **1982**, *382*, 471–482.
140. Bounds, D. G.; Klein, M. L.; McDonald, I. R.; Ozaki, Y. Static disorder in mixed crystals (KCN)<sub>x</sub>(KBr)<sub>1-x</sub> and its relationship to dynamical properties. *Mol. Phys.* **1982**, *47*, 629–636.
141. Nosé, S.; Klein, M. L. Molecular dynamics calculations for HCl in a matrix of solid Ar. *Mol. Phys.* **1982**, *46*, 1063–1071.
142. McDonald, I. R.; Bounds, D. G.; Klein, M. L. The disordered phases of potassium cyanide. *J. Phys. C: Solid State Phys.* **1983**, *16*, 3217–3232.
143. Tse, J. S.; Klein, M. L.; McDonald, I. R. Molecular dynamics studies of ice Ic and the structure I clathrate of methane hydrate. *J. Phys. Chem.* **1983**, *87*, 4198–4203.
144. Tse, J. S.; Klein, M. L.; McDonald, I. R. Dynamical properties of structure I clathrate hydrate of xenon. *J. Chem. Phys.* **1983**, *78*, 2096–2097.
145. O'Shea, S. F.; Ozaki, Y.; Klein, M. L. Vibrational amplitudes of xenon overlayers physisorbed on the graphite basal plane. *Chem. Phys. Lett.* **1983**, *94*, 355–358.
146. Goddard, J. D.; Klein, M. L.; Ozaki, Y. Ab initio interatomic potential curves for NaNO<sub>2</sub> and the simulation of the molten salt. *Proc. Phys. Soc. Jpn.* **1983**, *52*, 1168–1172.
147. Lynden-Bell, R. M.; McDonald, I. R.; Klein, M. L. Analysis of translation–rotation coupling in an orientationally disordered ionic crystal. *Mol. Phys.* **1983**, *48*, 1093–1117.
148. Nosé, S.; Klein, M. L. A study of solid liquid carbon tetrafluoride using the constant pressure molecular dynamics technique. *J. Chem. Phys.* **1983**, *78*, 6928–6939.
149. Nosé, S.; Klein, M. L. Structural transformations in solid nitrogen at high pressure. *Phys. Rev. Lett.* **1983**, *50*, 1207–1210.
150. Jorgensen, W. L.; Chandrasekhar, J.; Madura, J. D.; Impey, R. W.; Klein, M. L. Comparison of simple potential functions for simulating liquid water. *J. Chem. Phys.* **1983**, *79*, 926–935.
151. Fracassi, P. F.; Klein, M. L. Calculation of phonons in the pyrite phases of sodium superoxide. *Phys. Rev. B* **1983**, *28*, 997–1001.
152. Klein, M. L.; McDonald, I. R. Properties of solid potassium cyanide: Is the physics of cyanide crystals really chemistry? *J. Chem. Phys.* **1983**, *79*, 2333–2342.

153. Goddard, J. D.; Klein, M. L. Structure of the nitrite ion. *Phys. Rev. A* **1983**, 28, 1141–1143.
154. Levesque, D.; Weis, J. J.; Klein, M. L. New high-pressure phase of solid  $^4\text{He}$  is bcc. *Phys. Rev. Lett.* **1983**, 51, 670–673.
155. Klein, M. L.; McDonald, I. R.; Ozaki, Y. Orientational order in ionic crystals containing tetrahedral ions. *J. Chem. Phys.* **1983**, 79, 5579–5587.
156. Impey, R. W.; Nosé, S.; Klein, M. L. Polymorphic phase transitions in alkali cyanide crystals. *Mol. Phys.* **1983**, 50, 243–246.
157. Nosé, S.; Klein, M. L. Constant pressure molecular dynamics for molecular systems. *Mol. Phys.* **1983**, 50, 1055–1076.
158. Impey, R. W.; Klein, M. L. Intermolecular force models and the crystal structure of carbon disulfide. *Chem. Phys. Lett.* **1983**, 103, 143–146.
159. Joos, B.; Bergersen, B.; Klein, M. L. Ground state properties of xenon on graphite. *Phys. Rev. B* **1983**, 28, 7219–7224.
160. Tse, J.; Klein, M. L. Are hydrogen atoms solvated by water molecules? *J. Phys. Chem.* **1983**, 87, 5055–5057.
161. Vermesse, J.; Levesque, D.; Weis, J.-J.; Klein, M. L. Infrared absorption in doped rare gas crystals. *Can. J. Phys.* **1983**, 61, 1545–1548.
162. Fracassi, P. F.; Klein, M. L.; Della Vallee, R. G. Lattice dynamics of ionic molecular crystals in the rigid phases II and III of sodium superoxide. *Can. J. Phys.* **1984**, 62, 54–64.
163. Sprik, M.; Klein, M. L. A correlated variational wave function for the orientational ground state of solid methane. *J. Chem. Phys.* **1984**, 80, 1988–1999.
164. Klein, M. L.; O'Shea, S. F.; Ozaki, Y. Interaction potentials and the properties of xenon overlayers physisorbed on the graphite basal plane. *J. Phys. Chem.* **1984**, 88, 1420–1425.
165. Lynden-Bell, R. M.; Klein, M. L.; McDonald, I. R. Phonon orientational coupling in sodium nitrite. *Z. Phys. B: Condens. Matter* **1984**, 54, 325–331.
166. Impey, R. W.; Klein, M. L.; McDonald, I. R. Structure of the fast ion conducting phase of solid lithium sulfate. *J. Phys. C: Solid State Phys.* **1984**, 17, 3941–3944.
167. Neusy, E.; Nosé, S.; Klein, M. L. Molecular dynamics calculations for solid bicyclo (2.2.2) octane. *Mol. Phys.* **1984**, 52, 269–279.
168. DeRaedt, B.; Sprik, M.; Klein, M. L. Computer simulation of muonium in water. *J. Chem. Phys.* **1984**, 80, 5719–5724.
169. Sprik, M.; Impey, R. W.; Klein, M. L. Second-order elastic constants for the Lennard-Jones solid. *Phys. Rev.* **1984**, 29, 4368–4374.
170. Fracassi, P. F.; Klein, M. L. Translation–rotation coupling in the lattice dynamics of solid carbon monoxide. *Chem. Phys. Lett.* **1984**, 108, 359–362.
171. Nosé, S.; Klein, M. L. Molecular dynamics calculations for ethylene adsorbed on graphite. *Phys. Rev. Lett.* **1984**, 53, 818–821.
172. Marchese, M.; Jacucci, G.; Klein, M. L. Dispersion of surface phonons in a xenon monolayer physisorbed on the graphite basal plane. *Surf. Sci.* **1984**, 145, 364–370.
173. Tse, J. S.; Klein, M. L.; McDonald, I. R. Computer simulation studies of structure I clathrate hydrates of methane, tetrafluoromethane, cyclopropane and ethylene oxide. *J. Chem. Phys.* **1984**, 81, 6146–6153.
174. Sprik, M.; Klein, M. L. Orientational ordering in solid para-hydrogen and ortho-deuterium. *J. Chem. Phys.* **1984**, 81, 6207–6153.
175. Impey, R. W.; Klein, M. L.; Tse, J. S. Lattice vibrations of ices Ih, VIII, and IX. *J. Chem. Phys.* **1984**, 81, 6406–6407.
176. Impey, R. W.; Klein, M. L.; Tse, J. S. Effective pair potentials and the structure of ices VIII and IX. *J. Chem. Phys.* **1984**, 81, 6406–6407.
177. Impey, R. W.; Klein, M. L. A simple intermolecular potential for liquid ammonia. *Chem. Phys. Lett.* **1984**, 104, 579–582.
178. Fracassi, P. F.; Klein, M. L. Lattice dynamics of KCN and NaCN in their antiferro-electric phase III. *Can. J. Phys.* **1984**, 62, 725–729.
179. Cohen, S. S.; Klein, M. L. Dynamics of impure rare gas crystals. In *Inert Gases*; Klein, M. L., Ed.; Springer Series in Chemical Physics 34; Springer: New York, 1984; pp 87–144.
180. Klein, M. L. Computer simulations studies of solids. *Annu. Rev. Phys. Chem.* **1985**, 36, 525–548.
181. Impey, R. W.; Klein, M. L.; McDonald, I. R. Structural and dynamical properties of lithium sulfate in its solid electrolyte form. *J. Chem. Phys.* **1985**, 82, 4690–4698.
182. Sprik, M.; Klein, M. L.; Chandler, D. Staging: A sampling technique for the Monte Carlo evaluation path integrals. *Phys. Rev. B* **1985**, 31, 4234–4244.
183. Klein, M. L.; Impey, R. W. Computer simulation of molecular crystals. *J. Chim. Phys.* **1985**, 82, 111–115.
184. Cardini, G. G.; O'Shea, S. F.; Marchese, M.; Klein, M. L. Dispersion of surface phonons in xenon overlayers physisorbed on the Ag(111) surface. *Phys. Rev. B* **1985**, 32, 4261–4263.
185. Peters, C.; Klein, M. L. Monte Carlo calculations for solid CO and N<sub>2</sub> overlayers physisorbed on graphite. *Mol. Phys.* **1985**, 54, 895–909.
186. Sprik, M.; Klein, M. L.; Chandler, D. Computer simulation of an electron in a quenched disordered system: Observation of Lifshitz traps. *Phys. Rev. B* **1985**, 32, 545–547.
187. Fracassi, P. F.; Righini, R.; Della Valle, R. G.; Klein, M. L. Lattice dynamics of solid  $\alpha$ -carbon monoxide. *Chem. Phys.* **1985**, 96, 361–369.
188. Nosé, S.; Klein, M. L. Molecular dynamics study of the alloy (N<sub>2</sub>)<sub>67</sub>(Ar)<sub>29</sub>. *Can. J. Phys.* **1985**, 63, 1270–1273.
189. Sprik, M.; Klein, M. L.; Chandler, D. Simulation of an excess electron in a hard sphere fluid. *J. Chem. Phys.* **1985**, 83, 3042–3049.
190. Impey, R. W.; Sprik, M.; Klein, M. L. Simulation of the cubic to orthorhombic phase transition in potassium cyanide. *J. Chem. Phys.* **1985**, 83, 3638–3644.
191. Sprik, M.; Impey, R. W.; Klein, M. L. Study of electron solvation in liquid ammonia using quantum path integral Monte Carlo calculations. *J. Chem. Phys.* **1985**, 83, 5802–5809.
192. Impey, R. W.; Klein, M. L. Elastic constants of solid ammonia. *J. Chem. Phys.* **1985**, 83, 5346–5347.
193. Peters, C.; Klein, M. L. Structure of axially compressed monolayers of N<sub>2</sub> physisorbed on graphite. *Phys. Rev. B* **1985**, 32, 6077–6079.
194. Ferrario, M.; McDonald, I. R.; Klein, M. L. Structure of solid *t*-butyl cyanide: Interpretation of experimental data by means of molecular dynamics simulation. *J. Chem. Phys.* **1985**, 83, 4726–4733.

195. Cardini, G.; O'Shea, S. F.; Klein, M. L. Dynamics of physisorbed overlayers. *Faraday Discuss. Chem. Soc.* **1985**, 80, 227–238.
196. Sprik, M.; Impey, R. W.; Klein, M. L. Study of electron solvation in polar solvents using path integral calculations. *J. Stat. Phys.* **1986**, 43, 967–971.
197. Nosé, S.; Klein, M. L. Constant temperature—constant pressure molecular dynamics calculations for molecular solids: Application to solid nitrogen at high pressure. *Phys. Rev. B* **1986**, 33, 339–342.
198. Klein, M. L. Structure and dynamics of molecular crystals. In *Molecular Dynamics Simulation of Statistical-Mechanical Systems*; Ciccotti, G., Hoover, W., Eds.; North-Holland: Amsterdam, 1986; pp 424–476.
199. Ferrario, M.; McDonald, I. R.; Klein, M. L. Anion ordering in alkali cyanide crystals. *J. Chem. Phys.* **1986**, 84, 3975–3985.
200. Fracassi, P. F.; Cardini, G.; O'Shea, S. F.; Impey, R. W.; Klein, M. L. Solid and liquid carbon monoxide studied with the use of constant-pressure molecular dynamics. *Phys. Rev. B* **1986**, 33, 3441–3447.
201. Peters, C.; Morrison, J. A.; Klein, M. L. The adsorption of acetylene on a graphite surface. *Surf. Sci.* **1986**, 165, 355–374.
202. Sprik, M.; Impey, R. W.; Klein, M. L. Electron—ion interactions and ionization in a polar solvent. *Phys. Rev. Lett.* **1986**, 56, 2326–2329.
203. Ryckaert, J.-P.; Klein, M. L. Translational and rotational disorder in solid *n*-alkanes: Constant-pressure constant-temperature molecular dynamics calculations using infinitely long flexible chains. *J. Chem. Phys.* **1986**, 85, 1613–1620.
204. Marchi, M.; Tse, J. S.; Klein, M. L. Lattice vibrations and infrared absorption of ice Ih. *J. Chem. Phys.* **1986**, 85, 2414–2418.
205. Fowler, P. W.; Klein, M. L. Molecular properties of CN<sup>−</sup> ions in alkali cyanide crystals. *J. Chem. Phys.* **1986**, 85, 3913–3916.
206. Lynden-Bell, R. M.; Impey, R. W.; Klein, M. L. Investigation of the lattice vibrations of solid NaNO<sub>2</sub> by means of molecular dynamics calculation. *Chem. Phys.* **1986**, 109, 25–33.
207. Lewis, L. J.; Klein, M. L. Random strains and the structure of (KBr)<sub>1−x</sub>(KCN)<sub>x</sub> mixed crystals. *Phys. Rev. Lett.* **1986**, 57, 2698–2701.
208. Ryckaert, J.-P.; Klein, M. L.; McDonald, I. R. Disorder at the bilayer interface in the pseudo hexagonal rotator phase of solid *n*-alkanes. *Phys. Rev. Lett.* **1987**, 58, 698–701.
209. Tse, J. S.; Klein, M. L. Pressure induced phase transformations in ice. *Phys. Rev. Lett.* **1987**, 58, 1672–1675.
210. Lewis, L. J.; Klein, M. L. Quadrupolar freezing in (KBr)<sub>1−x</sub>(KCN)<sub>x</sub> mixed crystals. *J. Phys. Chem.* **1987**, 91, 4990–4994.
211. Impey, R. W.; Sprik, M.; Klein, M. L. Ionic solvation in non aqueous solvents: The structure of Li<sup>+</sup> and Cl<sup>−</sup> in methanol, ammonia, and methylamine. *J. Am. Chem. Soc.* **1987**, 109, 5900–5904.
212. Tse, J. S.; Klein, M. L. Dynamical properties of the structure II clathrate hydrate of krypton. *J. Phys. Chem.* **1987**, 91, 5789–5791.
213. Tse, J. S.; Klein, M. L. Molecular dynamics calculations of the infrared and Raman spectra of ice IX in the translation mode region. *Chem. Phys. Lett.* **1987**, 142, 175–180.
214. Sprik, M.; Klein, M. L. Optimization of a distributed gaussian basis set using simulated annealing: Application to the solvated electron. *J. Chem. Phys.* **1987**, 87, 5987–5999.
215. Ferrario, M.; Klein, M. L.; McDonald, I. R. Structure of solid *t*-butyl cyanide. A study by means of constant-pressure molecular dynamics simulation. *J. Chem. Phys.* **1987**, 87, 4823–4828.
216. Lewis, L. J.; Klein, M. L. Is the ground-state structure of (KCl)<sub>0.25</sub>(KCN)<sub>0.75</sub> a non-cubic orientational glass? *Phys. Rev. Lett.* **1987**, 59, 1837–1840.
217. Ferrario, M.; Klein, M. L.; Lynden-Bell, R. M.; McDonald, I. R. Molecular dynamics study of the rotator phase of *t*-butyl bromide. *J. Chem. Soc., Faraday Trans. 2* **1987**, 83, 2097–2111.
218. Klein, M. L. Intermolecular potentials and computer simulation studies of molecular crystals. *Stud. Phys. Theor. Chem.* **1987**, 46, 659–673.
219. Marchi, M.; Tse, J. S.; Klein, M. L. Infrared and raman spectrum of hexagonal ice in the lattice mode region. *J. Chem. Soc., Faraday Trans. 2* **1987**, 83, 1867–1874.
220. Klein, M. L.; Morrison, J. A. Gas—surface potentials and the interpretation of experiments on the ethylene/graphite system using molecular dynamics calculations. *Carbon* **1987**, 25, 23–30.
221. Klein, M. L.; Sprik, M. Adiabatic electron-ion recombination in a polar solvent. In *Chemical Reactivity in Liquids: Fundamental Aspects*; Moreau, M., Turq, P., Eds.; Plenum Press: New York, 1988; pp 175–186.
222. Marchi, M.; Sprik, M.; Klein, M. L. Solvation of electrons, atoms and ions in liquid ammonia. *Faraday Discuss. Chem. Soc.* **1988**, 85, 373–389.
223. Tse, J. S.; Klein, M. L. A molecular dynamics study of the effect of pressure on the properties of water and ice. *J. Phys. Chem.* **1988**, 92, 315–319.
224. Watanabe, K.; Ferrario, M.; Klein, M. L. Molecular dynamics study of a sodium octanoate micelle in aqueous solution. *J. Phys. Chem.* **1988**, 92, 819–821.
225. Cardini, G.; Bareman, J. P.; Klein, M. L. Characterization of a Langmuir—Blodgett monolayer using molecular dynamics calculations. *Chem. Phys. Lett.* **1988**, 145, 493–498.
226. Moller, M. A.; Klein, M. L. The low temperature structure of ethylene physisorbed on graphite. *Can. J. Chem.* **1988**, 66, 774–778.
227. Marchi, M.; Sprik, M.; Klein, M. L. Calculation of the free energy of electron solvation in liquid ammonia using path integral quantum Monte Carlo simulation. *J. Phys. Chem.* **1988**, 92, 3625–3629.
228. Bareman, J. P.; Cardini, G.; Klein, M. L. Characterization of structural and dynamical behavior in monolayers of long-chain molecules using molecular dynamics calculations. *Phys. Rev. Lett.* **1988**, 60, 2152–2154.
229. Demontis, P.; Le Sar, R.; Klein, M. L. New high pressure phases of ice. *Phys. Rev. Lett.* **1988**, 60, 2284–2287.
230. Sprik, M.; Klein, M. L. Application of path integral simulations to the study of electron solvation in polar fluids. *Comput. Phys. Rep.* **1988**, 7, 149–166.



231. Sprik, M.; Klein, M. L. Optimization of a distributed gaussian basis set using simulated annealing: Application to the adiabatic dynamics of the solvated electron. *J. Chem. Phys.* **1988**, *89*, 1592–1607. See erratum: Sprik, M.; Klein, M. L. *J. Chem. Phys.* **1989**, *90*, 7614.
232. Ruiz-Suarez, J. C.; Klein, M. L.; Moller, M.; Rowntree, P. A.; Scoles, G.; Xu, J. Structure of physisorbed overlayers of dipolar molecules: A combined study by helium beam scattering and molecular dynamics. *Phys. Rev. Lett.* **1988**, *61*, 710–713.
233. Marchi, M.; Sprik, M.; Klein, M. L. Electron attachment to ammonia clusters: A study using path integral Monte Carlo calculations. *J. Chem. Phys.* **1988**, *89*, 4918–4923.
234. Kuharski, R. A.; Bader, J. S.; Chandler, D.; Impey, R. W.; Sprik, M.; Klein, M. L. Molecular model for aqueous ferrous–ferric electron transfer. *J. Chem. Phys.* **1988**, *89*, 3248–3257.
235. Barrat, J.-L.; Roux, J.-N.; Hansen, J.-P.; Klein, M. L. Elastic response of a simple binary alloy near the glass transition. *Europhys. Lett.* **1988**, *7*, 707–712.
236. Yashonath, S.; Demontis, P.; Klein, M. L. Methane in zeolite NaY: A molecular dynamics study. *Chem. Phys. Lett.* **1988**, *153*, 551–556.
237. Sprik, M.; Klein, M. L. A polarizable model for water using distributed charge sites. *J. Chem. Phys.* **1988**, *89*, 7556–7560.
238. Forester, T. R.; McDonald, I. R.; Klein, M. L. Intermolecular potentials and properties of liquid and solid hydrogen sulphide. *Chem. Phys.* **1989**, *129*, 225–234.
239. Moller, M. A.; Klein, M. L. The continuous melting transition of ethylene on graphite. *Chem. Phys.* **1989**, *129*, 235–239.
240. Cardini, G.; Schettino, V.; Klein, M. L. Structure and dynamics of carbon dioxide clusters. *J. Chem. Phys.* **1989**, *90*, 4441–4449.
241. Watanabe, K.; Klein, M. L. Effective pair potentials and the properties of water. *Chem. Phys.* **1989**, *131*, 157–167.
242. Gamba, Z.; Klein, M. L. A molecular dynamics study of solid and liquid pyridine. *Chem. Phys.* **1989**, *130*, 15–22.
243. Moller, M. A.; Klein, M. L. A molecular dynamics study of the low-temperature structure and dynamics of ethane monolayers physisorbed on the graphite basal plane. *J. Chem. Phys.* **1989**, *90*, 1960–1967.
244. Ryckaert, J.-P.; McDonald, I. R.; Klein, M. L. Disorder in the pseudohexagonal rotator phase of *n*-alkanes: Molecular dynamics calculations for tricosane. *Mol. Phys.* **1989**, *67*, 957–979.
245. Nosé, S.; Klein, M. L. Structure and dynamics of the fluorperovskite,  $\text{RbCaF}_3$ . *J. Chem. Phys.* **1989**, *90*, 5005–5010.
246. Demontis, P.; Klein, M. L.; LeSar, R. High-density structures and phase transitions in an ionic model of ice. *Phys. Rev. B* **1989**, *40*, 2716–2718.
247. Demontis, P.; Yashonath, S.; Klein, M. L. Localization and mobility of benzene adsorption in sodium-Y zeolite. *J. Phys. Chem.* **1989**, *93*, 5016–5019.
248. Watanabe, K.; Klein, M. L. Shape fluctuations in ionic micelles. *J. Phys. Chem.* **1989**, *93*, 6837–6901.
249. Barrat, J. L.; Loubeyre, P.; Klein, M. L. Isotopic shift in the melting curve of helium: A path integral Monte Carlo study. *J. Chem. Phys.* **1989**, *90*, 5644–5650.
250. Marchi, M.; Klein, M. L. A computer simulation study of supercooled and amorphous-solid methanol. *Z. Naturforsch., A: Phys. Sci.* **1989**, *44*, 585–590.
251. Sprik, M.; Klein, M. L. Adiabatic dynamics of the solvated electron in liquid ammonia. *J. Chem. Phys.* **1989**, *91*, 5665–5671.
252. Lewis, L. J.; Klein, M. L. Molecular-dynamics studies of the mixed cyanides I: Structural transformations. *Phys. Rev.* **1989**, *40*, 4877–4888.
253. Hautman, J.; Klein, M. L. Simulation of a monolayer of alkyl thiol chains. *J. Chem. Phys.* **1989**, *91*, 4994–5001.
254. Lewis, L. J.; Klein, M. L. Molecular-dynamics studies of mixed cyanides. II. Orientation freezing. *Phys. Rev. B* **1989**, *40*, 7080–7090.
255. Lewis, L. J.; Klein, M. L. Structural transitions in the heavily-strained cyanide crystal  $(\text{KCl})_{0.25}(\text{KCN})_{0.75}$ . *Phys. Rev. B* **1989**, *40*, 7904–7911.
256. Sindzingre, P.; Klein, M. L.; Ceperley, D. M. Path integral Monte Carlo study of low-temperature  $^4\text{He}$  clusters. *Phys. Rev. Lett.* **1989**, *63*, 1601–1604.
257. Klein, M. L.; Demontis, P. Molecular dynamics for systems under high pressure. In *Simple Molecular Systems at Very High Density*; Polian, A., Loubeyre, P., Boccara, N., Eds.; Plenum Press: New York, 1989; pp 441–454.
258. Bareman, J. P.; Cardini, G.; Klein, M. L. Molecular dynamics study of a model Langmuir–Blodgett film. *Mater. Res. Soc. Symp. Proc.* **1989**, *141*, 411–418.
259. Ryckaert, J. P.; McDonald, I. R.; Klein, M. L. Use of an all-atom, semi-flexible model in molecular dynamics simulation of long-chain paraffins. In *Computer Simulation of Polymers*; Roe, R. J., Ed.; Prentice Hall: Englewood Cliffs, NJ, 1990; pp 70–77.
260. Shelley, J.; Watanabe, K.; Klein, M. L. Simulation of a sodium dodecylsulphate micelle in aqueous solution. *Int. J. Quantum Chem., Quantum Biol. Symp.* **1990**, *17*, 102–117.
261. Marchi, M.; Sprik, M.; Klein, M. L. Calculation of the molar volume of electron solvation in ammonia. *J. Phys. Chem.* **1990**, *94*, 431–434.
262. Signorini, G.; Barrat, J.-L.; Klein, M. L. Structural relaxation and dynamical correlations in a molten salt near the liquid–glass transition: A molecular dynamics study. *J. Chem. Phys.* **1990**, *92*, 1294–1303.
263. Gamba, Z.; Klein, M. L. Short-range structure of liquid pyrrole. *J. Chem. Phys.* **1990**, *92*, 6973–6974.
264. Sprik, M.; Klein, M. L.; Watanabe, K. Solvent polarization and hydration of the chloride anion. *J. Phys. Chem.* **1990**, *94*, 6483–6488.
265. Tse, J. S.; Klein, M. L. Pressure-induced amorphization of ice  $\text{I}_h$ . *J. Chem. Phys.* **1990**, *92*, 3992–3994.
266. Marchi, M.; Sprik, M.; Klein, M. L. Solvation and ionization of alkali metals in liquid ammonia: A path integral Monte Carlo study. *J. Phys.: Condens. Matter* **1990**, *2*, 5833–5848.
267. Bareman, J. P.; Klein, M. L. Collective tilt behavior in monolayers of long-chain molecules: A molecular dynamics study. *J. Phys. Chem.* **1990**, *94*, 5202–5205.
268. Hautman, J.; Klein, M. L. Molecular dynamics simulation of the effect of temperature on the behavior of dense monolayers of long-chain molecules. *J. Chem. Phys.* **1990**, *93*, 7483–7492.

269. Ferrario, M.; Haughney, M.; McDonald, I. R.; Klein, M. L. Molecular dynamics simulation of aqueous mixtures: Methanol, acetone and ammonia. *J. Chem. Phys.* **1990**, *93*, 5156–5166.
270. Lewis, L. J.; Klei, M. L. Computer simulation of dynamical properties of bulk solids. In *Dynamical Properties of Solids*; Horton, G. K., Maradudin, A. A., Eds.; North Holland: Amsterdam, 1990; Vol. 6, Chapter 7, pp 383–492.
271. Klein, M. L.; Lewis, L. J. Simulation of dynamical processes in molecular solids. *Chem. Rev.* **1990**, *90*, 459–479.
272. Barrat, J.-L.; Klein, M. L. Molecular dynamics simulations of supercooled liquids near the glass transition. *Annu. Rev. Phys. Chem.* **1991**, *42*, 23–53.
273. Martyna, G.; Klein, M. L. Pseudopotential calculation of the electronic states of small metal–ammonia clusters. *J. Phys. Chem.* **1991**, *95*, 515–518.
274. Cheng, A.; Klein, M. L.; Lewis, L. Competing interactions and orientational ordering in  $(\text{NaCN})_{1-x}(\text{KCN})_x$  quadrupolar glasses. *Phys. Rev. Lett.* **1991**, *95*, 624–627.
275. Watanabe, K.; Klein, M. L. Molecular dynamics studies of the system sodium octanoate and water: The liquid crystal mesophase with two-dimensional hexagonal symmetry. *J. Phys. Chem.* **1991**, *95*, 4158–4166.
276. Cheng, A.; Klein, M. L.; Lewis, L. Orientational ordering in mixed cyanide crystals:  $(\text{NaCN})_{1-x}(\text{KCN})_x$ . *Phys. Rev. B* **1991**, *44*, 13–22.
277. Martyna, G.; Cheng, C.; Klein, M. L. Electronic states and dynamical behavior of  $\text{LiXe}_n$  and  $\text{CsXe}_n$  clusters. *J. Chem. Phys.* **1991**, *95*, 1318–1336.
278. Yashonath, S.; Klein, M. L. Temperature and concentration dependence of adsorption properties of methane in zeolite-NaY: A molecular dynamics study. *J. Phys. Chem.* **1991**, *95*, 5881–5889.
279. Cheng, A.; Klein, M. L. Molecular dynamics simulation of solid buckminsterfullerenes. *J. Phys. Chem.* **1991**, *95*, 6750–6751.
280. Cowley, E. Roger; Klein, M. L. A molecular dynamics study of lattice vibrations in the mixed crystal  $\text{K}_{0.5}\text{Rb}_{0.5}\text{Cl}$ . *Phys. Rev. B* **1991**, *44*, 5000–5006.
281. Sindzingre, Ph.; Ceperley, D. M.; Klein, M. L. Superfluidity in clusters of para- $\text{H}_2$  molecules. *Phys. Rev. Lett.* **1991**, *67*, 1871–1874.
282. Cheng, A.; Klein, M. L. Molecular dynamics investigations of alkali-doped fullerenes. *J. Phys. Chem.* **1991**, *95*, 9622–9625.
283. Hautman, J.; Klein, M. L. Microscopic wetting phenomena. *Phys. Rev. Lett.* **1991**, *67*, 1763–1766.
284. Hautman, J.; Bareman, J. P.; Mar, W.; Klein, M. L. Molecular dynamics investigations of self-assembled monolayers. *J. Chem. Soc., Faraday Trans.* **1991**, *87*, 2031–2037.
285. Shelley, J.; Watanabe, K.; Klein, M. L. Simulation of sodium octanoate micelles in aqueous solution. *Electrochim. Acta* **1991**, *36*, 1729–1734.
286. Hautman, J.; Klein, M. Structural organization in self-assembled monolayers. In *Computer Simulation in Materials Science*; Meyer, M., Pontikis, V., Eds.; Kluwer: Boston, MA, 1991; pp 395–405.
287. Martyna, G.; Klein, M. L. Path integral studies of metal–ammonia clusters and solution. *J. Phys. IV* **1991**, *C5*, 103–113.
288. Klein, M. L. Conformations of flexible molecules in fluid phases. *J. Chem. Soc., Faraday Trans.* **1992**, *88*, 1701–1705.
289. Hautman, J.; Klein, M. L. Simulation of microscopic wetting phenomena on self-assembled monolayers. *Mater. Res. Soc. Symp. Proc.* **1992**, *237*, 303–310.
290. Klein, M. L. Computer simulation of micelles in aqueous solution. In *Structure and Dynamics of Strongly Interacting Colloids and Supramolecular Aggregates in Solution*; Chen, S. H., Huang, J. S., Tartaglia, P., Eds.; NATO ASI Series, Series C, Mathematical and Physical Sciences 369; Kluwer: Boston, MA, 1992; pp 511–518.
291. Bareman, J. P.; Klein, M. L. Molecular dynamics simulation of a Langmuir monolayer. *Mater. Res. Soc. Symp. Proc.* **1992**, *237*, 271–279.
292. Sindzingre, P.; Klein, M. L. A molecular dynamics study of methanol near the liquid–glass transition. *J. Chem. Phys.* **1992**, *96*, 4681–4692.
293. Cheng, A.; Klein, M. L.; Parrinello, M.; Sprik, M. Intermolecular interactions and the nature of orientational ordering in the solid fullerenes  $\text{C}_{60}$  and  $\text{C}_{70}$ : Predictions from molecular dynamics calculations. *Philos. Trans. R. Soc. London, Ser. A* **1992**, *341*, 327–336.
294. Martyna, G. J.; Klein, M. L. The electronic states of lithium atoms in ammonia clusters and solution. *J. Chem. Phys.* **1992**, *96*, 7662–7671.
295. Cheng, A.; Klein, M. L. Molecular dynamics investigation of orientational freezing in solid  $\text{C}_{60}$ . *Phys. Rev. B* **1992**, *45*, 1889–1895.
296. Sprik, M.; Cheng, A.; Klein, M. L. Modeling the orientational ordering transition in solid  $\text{C}_{60}$ . *J. Phys. Chem.* **1992**, *96*, 2027–2029.
297. Deng, Z.; Martyna, G.; Klein, M. L. Structure and dynamics of bipolarons in liquid ammonia. *Phys. Rev. Lett.* **1992**, *68*, 2496–2499.
298. Scharf, D.; Martyna, G. J.; Klein, M. L. Path-integral Monte Carlo studies of para-hydrogen clusters. *J. Chem. Phys.* **1992**, *97*, 3590–3599.
299. Cheng, A.; Klein, M. L. Solid  $\text{C}_{70}$ : A molecular dynamics investigation of structure and orientational ordering. *Phys. Rev. B* **1992**, *46*, 4958–4962.
300. Sprik, M.; Cheng, A.; Klein, M. L. Orientational ordering in solid  $\text{C}_{70}$ : Predictions from computer simulation. *Phys. Rev. Lett.* **1992**, *69*, 1660–1663.
301. Cheng, A.; Klein, M. L.  $\text{C}_{60}\text{O}$ : A molecular study of molecular rotation in the solid phase. *J. Chem. Soc., Faraday Trans.* **1992**, *88*, 1949–1951.
302. Martyna, G.; Klein, M. L.; Tuckerman, M. Nosé–Hoover chains: The canonical ensemble via continuous dynamics. *J. Chem. Phys.* **1992**, *97*, 2635–2643.
303. Scharf, D.; Martyna, G.; Klein, M. L. Isotope effect on the melting of para-hydrogen and ortho-deuterium clusters. *Chem. Phys. Lett.* **1992**, *197*, 231–235.
304. Cheng, A.; Klein, M. L. Melting of ethylene on graphite. *Langmuir* **1992**, *8*, 2798–2803.
305. Gamba, Z.; Hautman, J.; Klein, M. L. Molecular dynamics simulation of a Newton black film. *Langmuir* **1992**, *8*, 3155–3160.
306. Hautman, J.; Klein, M. L. An Ewald summation method for planar surfaces and interfaces. *Mol. Phys.* **1992**, *75*, 379–395.



307. Cheng, A.; Klein, M. L.; Parrinello, M.; Sprik, M. Intermolecular interactions and the nature of orientational ordering in the solid fullerenes C<sub>60</sub> and C<sub>70</sub>: Predictions from molecular dynamics calculation. In *New Methods for Modeling Processes within Solids and at Their Surfaces*; Catlow, C. R. A., Stoneham, A. M., Thomas, J. M., Eds.; Oxford: New York, 1993; pp 133–142.
308. Martyna, G. J.; Deng, Z.; Klein, M. L. Quantum simulation studies for singlet and triplet state bipolarons in liquid ammonia. *J. Chem. Phys.* **1993**, *98*, 555–563.
309. Tobias, D.; Klein, M. L.; Opella, S. J. Molecular dynamics simulation of Pf1 coat protein. *Biophys. J.* **1993**, *64*, 670–675.
310. Shelley, J. C.; Sprik, M.; Klein, M. L. Simulation of an aqueous sodium octanoate micelle using polarizable surfactant molecules. *Langmuir* **1993**, *9*, 916–926.
311. Deng, Z.; Martyna, G. J.; Klein, M. L. Electronic states in metal–ammonia solutions. *Phys. Rev. Lett.* **1993**, *71*, 267–270.
312. Scharf, D.; Martyna, G. J.; Klein, M. L. Structure and energetics of fluid para-hydrogen. *Fiz. Nizk. Temp.* **1993**, *19*, 516–519.
313. Hautman, J.; Klein, M. L. Effects of particle size fluctuations in a breathing Lennard-Jones fluid. *Mol. Phys.* **1993**, *80*, 647–654.
314. Scharf, D.; Martyna, G. J.; Liu, D.; Voth, G. A.; Klein, M. L. Nature of the lithium trapping sites in the quantum solids para-hydrogen and ortho-deuterium. *J. Chem. Phys.* **1993**, *99*, 9013–9020.
315. Scharf, D.; Martyna, G. J.; Klein, M. L. Path integral Monte Carlo study of a lithium impurity in para-hydrogen: Clusters and the bulk liquid. *J. Chem. Phys.* **1993**, *99*, 8997–9012.
316. Tobias, D.; Martyna, G. J.; Klein, M. L. Molecular dynamics simulations of a protein in the canonical ensemble. *J. Phys. Chem.* **1993**, *97*, 12959–12966.
317. Ferrario, M.; McDonald, I. R.; Klein, M. L. Dynamical behavior of the azide ion in protic solvents. *Chem. Phys. Lett.* **1993**, *213*, 537–540.
318. Mar, W.; Hautman, J.; Klein, M. L. Molecular dynamics studies of microscopic wetting phenomena. *Tenside, Surfactants, Deterg.* **1993**, *30*, 252–255.
319. Cheng, A.; Klein, M. L.; Caccamo, C. Prediction of the phase diagram of rigid C<sub>60</sub> molecules. *Phys. Rev. Lett.* **1993**, *71*, 1200–1203.
320. Tuckerman, M. E.; Berne, B. J.; Martyna, G. J.; Klein, M. L. Efficient molecular dynamics and hybrid Monte Carlo algorithms for path integrals. *J. Chem. Phys.* **1993**, *99*, 2796–2808.
321. Mar, W.; Klein, M. L. Molecular dynamics study of self-assembled alkylthiol monolayers using an all-atoms model. *Langmuir* **1994**, *10*, 188–196.
322. Gamba, Z.; Klein, M. L. Simple models of the intermolecular potential for the condensed phases of C<sub>60</sub>. *Condens. Matter Theor.* **1993**, *8*, 535–542.
323. Röthlisberger, U.; Klein, M. L.; Sprik, M. Competing interactions in self-assembled monolayers containing peptide groups: Molecular dynamics studies of long-chain perfluoro mercaptans on Au(111). *J. Mater. Chem.* **1994**, *4*, 793–803.
324. Martyna, G. J.; Tobias, D.; Klein, M. L. Constant pressure molecular dynamics algorithms. *J. Chem. Phys.* **1994**, *101*, 4177–4187.
325. Deng, Z.; Martyna, G. J.; Klein, M. L. Quantum simulation studies of metal–ammonia solutions. *J. Chem. Phys.* **1994**, *100*, 7590–7601.
326. Kohanoff, J.; Buda, F.; Parrinello, M.; Klein, M. L. Nature of the conduction states in the metallic molecular crystal Li(NH<sub>3</sub>)<sub>4</sub>. *Phys. Rev. Lett.* **1994**, *73*, 3133–3136.
327. Deng, Z.; Martyna, G. J.; Klein, M. L. Electronic states and the metal–insulator transition in cesium–ammonia solutions. *J. Chem. Soc., Faraday Trans.* **1994**, *90*, 2009–2013.
328. Cardini, G.; Bini, R.; Salvi, P.; Schettino, V.; Klein, M. L.; Strongin, R. M.; Brard, L.; Smith, A., III. Infrared spectrum of two fullerene derivatives: C<sub>60</sub>O and C<sub>61</sub>H<sub>2</sub>. *J. Phys. Chem.* **1994**, *98*, 9966–9971.
329. Mar, W.; Klein, M. L. A molecular dynamics study of n-hexadecane droplets on a hydrophobic surface. *J. Phys.: Condens. Matter* **1994**, *6*, A381–A388.
330. Laasonen, K.; Klein, M. L. Structural study of (H<sub>2</sub>O)<sub>20</sub> and (H<sub>2</sub>O)<sub>21</sub>H<sup>+</sup> using density functional methods. *J. Phys. Chem.* **1994**, *98*, 10079–10083.
331. Seipmann, J. I.; Karaborni, S.; Klein, M. L. Monte Carlo simulations of liquid–vapor coexistence in Langmuir monolayer of pentadecanoic acid. *J. Phys. Chem.* **1994**, *98*, 6675–6678.
332. Sprik, M.; Klein, M. L. Intermolecular motion in solid C<sub>70</sub>: A molecular dynamics study. *J. Phys. Chem.* **1994**, *98*, 9297–9300.
333. Sprik, M.; Delmarche, E.; Michel, B.; Röthlisberger, U.; Klein, M. L.; Wolf, H.; Ringsdorf, H. The structure of hydrophilic self-assembled monolayers: A combined scanning tunneling microscopy and computer simulation study. *Langmuir* **1994**, *10*, 4116–4130.
334. Ryckaert, J.-P.; Klein, M. L.; McDonald, I. R. Computer simulations and the interpretation of incoherent neutron scattering experiments on the solid rotator phases of long-chain alkanes. *Mol. Phys.* **1994**, *83*, 439–458.
335. Röthlisberger, U.; Klein, M. L. The performance of density-functional methods for the description of weak interaction potentials: The butane torsional potential. *Chem. Phys. Lett.* **1994**, *227*, 390–395.
336. Laasonen, K.; Klein, M. L. Ab initio molecular dynamics study of hydrochloric acid in water. *J. Am. Chem. Soc.* **1994**, *116*, 11620–11621.
337. Cheng, A.; Klein, M. L. Orientational ordering in the solid fullerene oxide: C<sub>60</sub>O. *J. Chem. Soc., Faraday Trans.* **1994**, *90*, 253–261.
338. Scharf, D.; Martyna, G. J.; Klein, M. L. Electronic spectra of a lithium impurity in clusters, the bulk liquid, and solid para-hydrogen. In *Reaction Dynamics in Clusters and Condensed Phases*; Jortner, J., Pullman, B., Levine, R. D., Eds.; The Jerusalem Symposia on Quantum Chemistry and Biochemistry 26; Kluwer: Dordrecht, The Netherlands, 1994; pp 153–168.
339. Röthlisberger, U.; Klein, M. L.; Sprik, M. Simulation of self-assembled monolayers: Microscopic structure of amino-alkylthiols. In *Computational Approaches in Supramolecular Chemistry*; Wipff, G., Ed.; Kluwer: Dordrecht, The Netherlands, 1994; pp 399–409.
340. Deng, Z.; Martyna, G. J.; Klein, M. L. Quantum simulation studies of bipolarons in cesium–ammonia solutions. In *Toward Teraflop Computing and New Grand Challenge Applications*; Kalia, R. K., Vashista, P., Eds.; Nova: New York, 1994.

341. Hautman, J.; Klein, M. L. Domains and superlattices in self-assembled monolayers of long-chain molecules. In *Theoretical and Computational Approaches to Interface Phenomena*; Sellers, H., Ed.; Plenum: New York, 1994; pp 149–159.
342. Laasonen, K. E.; Klein, M. L. Molecular dynamics simulations of the structure and ion diffusion in PEO. *J. Chem. Soc., Faraday Trans.* **1995**, *91*, 2633–2638.
343. Ferrario, M.; Klein, M. L.; McDonald, I. R. Cation transport in lithium-sulphate-based crystals. *Mol. Phys.* **1995**, *86*, 923–938.
344. Seitsonen, A. P.; Laasonen, K.; Nieminen, R. M.; Klein, M. L. Structure of  $\text{CaI}_{12}$ . *J. Chem. Phys.* **1995**, *103*, 8075–8080.
345. Röthlisberger, U.; Klein, M. L. Ab initio molecular dynamics investigation of singlet  $\text{C}_2\text{H}_2\text{Li}_2$ : Determination of the ground-state structure and observation of LiH intermediates. *J. Am. Chem. Soc.* **1995**, *117*, 42–48.
346. Tu, K.; Tobias, D. J.; Klein, M. L. Constant pressure and temperature molecular dynamics simulations of the lecithin fragments: Glycerylphosphorylcholine and dilauroylglycerol. *J. Phys. Chem.* **1995**, *99*, 10035–10042.
347. Mar, W.; Hautman, J.; Klein, M. L. Molecular dynamics study of microscopic wetting phenomena on self-assembled monolayers. *Comput. Mater. Sci.* **1995**, *3*, 481–497.
348. Mundy, C. J.; Siepmann, J. I.; Klein, M. L. Calculation of the shear viscosity of decane using a reversible multiple time-step algorithm. *J. Chem. Phys.* **1995**, *102*, 3376–3380.
349. Tarek, M.; Tobias, D. J.; Klein, M. L. Molecular dynamics simulation of tetradecyltrimethylammonium bromide monolayers at the air/water interface. *J. Phys. Chem.* **1995**, *99*, 1393–1402.
350. Ungar, P. J.; Laasonen, K. E.; Klein, M. L. Ab initio simulation of the structure and dynamics of white phosphorous ( $\text{P}_4$ ) at low temperature. *Can. J. Phys.* **1995**, *73*, 710–717.
351. Tu, K.; Tobias, D. J.; Klein, M. L. Constant pressure and temperature molecular dynamics simulation of the fully-hydrated liquid-crystal phase of dipalmitoyl-phosphatidylcholine. *Biophys. J.* **1995**, *69*, 2558–2562.
352. Balasubramanian, S.; Klein, M. L.; Siepmann, J. I. Monte Carlo investigations of hexadecane films on a metal substrate. *J. Chem. Phys.* **1995**, *103*, 3184–3195.
353. Tobias, D. J.; Gesell, J.; Klein, M. L.; Opella, S. J. A simple protocol for identification of helical and mobile residues in membrane proteins. *J. Mol. Biol.* **1995**, *253*, 391–395.
354. Mundy, C. J.; Siepmann, J. I.; Klein, M. L. Decane under shear: A molecular dynamics study using reversible NVT-SLLOD and NPT-SLLOD algorithms. *J. Chem. Phys.* **1995**, *103*, 10192–10200.
355. Tobias, D. J.; Klein, M. L. Molecular dynamics investigation of the lamella liquid-crystal d-phase in the octylammonium chloride /water system. *Mol. Simul.* **1996**, *16*, 219–228.
356. Tuckerman, M. E.; Marx, D.; Klein, M. L.; Parrinello, M. Efficient and general algorithms for path integral Car–Parrinello molecular dynamics. *J. Chem. Phys.* **1996**, *104*, 5579–5588.
357. Tobias, D. J.; Klein, M. L. Molecular dynamics investigation of a calcium carbonate/calcium sulfonate reverse micelle. *J. Phys. Chem.* **1996**, *100*, 6637–6648.
358. Tu, K.; Tobias, D. J.; Blasie, J. K.; Klein, M. L. Molecular dynamics simulation of the fully-hydrated bilayer gel-phase of dipalmitoyl-phosphatidylcholine. *Biophys. J.* **1996**, *70*, 595–608.
359. Martyna, G. J.; Tuckerman, M. E.; Tobias, D. J.; Klein, M. L. Explicit reversible integrators for extended system dynamics. *Mol. Phys.* **1996**, *87*, 1117–1157.
360. Sagnella, D. E.; Laasonen, K.; Klein, M. L. Molecular dynamics studies of proton transfer in a poly-glycine analog of the ion channel gramicidin A. *Biophys. J.* **1996**, *71*, 1172–1178.
361. Balasubramanian, S.; Klein, M. L.; Siepmann, J. I. Simulation studies of ultrathin films of linear and branched alkanes on a metal substrate. *J. Phys. Chem.* **1996**, *100*, 11960–11963.
362. Tobias, D. J.; Tu, K.; Klein, M. L. Molecular dynamics simulation of lipid bilayers. In *Monte Carlo and Molecular Dynamics of Condensed Systems*; Binder, K., Ciccotti, G., Eds.; SIF: Bologna, Italy, 1996; pp 327–344.
363. Röthlisberger, U.; Laasonen, K. E.; Klein, M. L.; Sprik, M. The torsional potential of perfluoro *n*-alkanes: A density functional study. *J. Chem. Phys.* **1996**, *104*, 3692–3700.
364. Laasonen, K.; Klein, M. L. Ab initio molecular dynamics study of dilute hydrofluoric acid. *Mol. Phys.* **1996**, *88*, 135–142.
365. Tarek, M.; Tobias, D. J.; Klein, M. L. Molecular dynamics investigation of the surface/bulk equilibrium in an ethanol–water solution. *J. Chem. Soc., Faraday Trans.* **1996**, *92*, 559–563.
366. Tuckerman, M. E.; Unger, P. J.; von Rosenvigne, T.; Klein, M. L. Ab initio molecular dynamics simulations. *J. Phys. Chem.* **1996**, *100*, 12878–12887.
367. Okada, O.; Klein, M. L. Molecular dynamics studies of titanilphthalocyanine crystals. *J. Chem. Soc., Faraday Trans.* **1996**, *92*, 2463–2467.
368. Tuckerman, M. E.; von Rosenvigne, T.; Klein, M. L. Ab initio molecular dynamics simulations of molecular crystals. *Mater. Res. Soc. Symp. Proc.* **1996**, *408*, 477–488.
369. Tobias, D. J.; Mar, W.; Blasie, J. K.; Klein, M. L. Molecular dynamics simulation of a protein on hydrophobic and hydrophilic surfaces: Cytochrome c on methyl and thiol terminated self-assembled monolayers. *Biophys. J.* **1996**, *71*, 2933–2941.
370. Tarek, M.; Tobias, D. J.; Klein, M. L. Molecular dynamics investigation of an ethanol–water solution. *Physica A* **1996**, *2839*, 559–563.
371. Mundy, C. J.; Balasubramanian, S.; Klein, M. L. Hydrodynamic boundary conditions for confined fluids via a non-equilibrium molecular dynamics simulation. *J. Chem. Phys.* **1996**, *105*, 3211–3214.
372. Balasubramanian, S.; Mundy, C. J.; Klein, M. L. The shear viscosity of polar fluids: Molecular dynamics calculations for water. *J. Chem. Phys.* **1996**, *105*, 11190–11195.
373. Bagchi, K.; Mundy, C. J.; Balasubramanian, S.; Klein, M. L. Profile unbiased thermostat with dynamical streaming velocities. *J. Chem. Phys.* **1996**, *105*, 11183–11189.
374. Mundy, C. J.; Klein, M. L.; Siepmann, J. I. Determination of the pressure–viscosity coefficient of decane by molecular simulation. *J. Phys. Chem.* **1996**, *100*, 16779–16781.

375. Stoneham, M.; Klein, M. L. Modelling and simulation of solids. *Solid State Mater. Sci.* **1996**, *1*, 817–819.
376. Kung, P. W. C.; Books, J. T.; Freeman, C. M.; Levine, S. M.; Vessal, B.; Newsam, J. M.; Klein, M. L. Melting of aromatic compounds: Molecular dynamics simulations. *Mater. Res. Soc. Symp. Proc.* **1996**, *408*, 327–332.
377. Mundy, C. J.; Balasubramanian, S.; Bagchi, K.; Klein, M. L.; Siepmann, J. I. Equilibrium and non-equilibrium simulation studies of complex fluids at interfaces. *Faraday Discuss.* **1996**, *104*, 17–36.
378. Laasonen, K.; Klein, M. L. Ab initio molecular dynamics study of aqueous hydrochloric acid solutions. *J. Phys. Chem. A* **1997**, *101*, 98–102.
379. Siepmann, J. I.; Martin, M. G.; Mundy, C. J.; Klein, M. L. Intermolecular potentials for branched alkanes and the vapor–liquid-phase equilibria for *n*-heptane, 2-methylhexane, and 3-ethylpentane. *Mol. Phys.* **1997**, *90*, 687–693.
380. Mundy, C. J.; Balasubramanian, S.; Klein, M. L. Computation of the hydrodynamic dynamics boundary parameters of a confined fluid via non-equilibrium molecular dynamics. *Physica A* **1997**, *240*, 305–331.
381. Tuckerman, M. E.; Mundy, C. J.; Klein, M. L. Toward a statistical mechanics of steady states. *Phys. Rev. Lett.* **1997**, *78*, 2042–2045.
382. Tuckerman, M. E.; Marx, D.; Klein, M. L.; Parrinello, M. Quantum character of a proton in a hydrogen bond. *Science* **1997**, *275*, 817–820.
383. Sprik, M.; Röthlisberger, U.; Klein, M. L. Structure of solid poly(tetrafluoroethylene): A computer simulation study of chain conformational, translational and orientational disorder. *J. Phys. Chem.* **1997**, *101*, 2745–2749.
384. Kinugawa, K.; Moore, P. B.; Klein, M. L. Centroid path integral molecular dynamics simulation of lithium para-hydrogen clusters. *J. Chem. Phys.* **1997**, *106*, 1154–1169.
385. Klein, M. L.; Marchi, M.; Smith, J. C. Potential functions for simulation of biomolecular systems. *J. Chim. Phys.* **1997**, *94*, 1305–1312.
386. von Rosenvigne, T.; Parrinello, M.; Klein, M. L. Ab initio studies of polyfluoride anions. *J. Chem. Phys.* **1997**, *107*, 8012–8019.
387. Tobias, D. J.; Tu, K.; Klein, M. L. Atomic-scale molecular dynamics simulation of lipid membranes. *Curr. Opin. Colloid Interface Sci.* **1997**, *2*, 15–26.
388. Shelley, J. C.; Sprik, M.; Klein, M. L. Structure and electrostatics of the surfactant–water interface. *Prog. Colloid Polym. Sci.* **1997**, *103*, 146–154.
389. Tuckerman, M. E.; Mundy, C. J.; Balasubramanian, S.; Klein, M. L. Modified nonequilibrium molecular dynamics for fluid flows with energy conservation. *J. Chem. Phys.* **1997**, *106*, 5615–5621.
390. Tarek, M.; Klein, M. L. Molecular dynamics study of two-component systems: The shape and surface structure of water/ethanol droplets. *J. Phys. Chem. A* **1997**, *101*, 8639–8642.
391. Zhong, Q.; Husslein, T.; Klein, M. L. Ion channels a challenge for computer simulations. In *Classical and Quantum Dynamics in Condensed Phase Simulations*; Berne, B. J., Ciccotti, G., Coker, D. F., Eds.; World Scientific: Singapore, 1998; pp 463–486.
392. Bagchi, K.; Balasubramanian, S.; Klein, M. L. The effect of pressure on the properties of water: Molecular dynamics calculations for the extended point-charge model. *J. Chem. Phys.* **1997**, *107*, 8561–8567.
393. Tobias, D. J.; Tu, K.; Klein, M. L. Assessment of all-atom potentials for modeling membranes: Molecular dynamics simulations of solid and liquid alkanes and crystals of phospholipid fragments. *J. Chim. Phys.* **1997**, *94*, 1482–1502.
394. von Rosenvigne, T.; Tuckerman, M. E.; Klein, M. L. Ab initio molecular dynamics studies of acid hydrates. *Faraday Discuss.* **1997**, *106*, 273–289.
395. *Physics of Cryocrystals*; Manzhelii, V. G., Freiman, Y. A., Eds. (English language version, Klein, M. L., Maradudin, A. A., Eds.); American Institute of Physics: Woodbury, NY, 1997.
396. Röthlisberger, U.; Sprik, M.; Klein, M. L. Living polymers: Ab initio investigation of the initiation step in the polymerization of isoprene induced by ethyl lithium. *J. Chem. Soc., Faraday Trans.* **1998**, *94*, 501–508.
397. Zhong, Q.; Jiang, Q.; Moore, P. M.; Newns, D. M.; Klein, M. L. Molecular dynamics simulation of a synthetic ion channel. *Biophys. J.* **1998**, *74*, 3–10.
398. Alivisatos, A. P.; Barbara, P. F.; Castleman, A. W.; Chang, J.; Dixon, D. A.; Klein, M. L.; McLendon, G. L.; Miller, J. S.; Ratner, M. A.; Rossky, P. J.; Stupp, S. I.; Thompson, M. From molecules to materials: Current trends and future directions. *Adv. Mater.* **1998**, *10*, 1297–1336.
399. Zhong, Q.; Moore, P. M.; Newns, D. M.; Klein, M. L. Molecular dynamics study of the LS3 voltage-gated ion channel. *FEBS Lett.* **1998**, *427*, 267–270.
400. Tarek, M.; Bandyopadhyay, S.; Klein, M. L. Molecular dynamics studies of aqueous surfactant system. *J. Mol. Liq.* **1998**, *78*, 1–6.
401. Woska, A. B.; Klein, M. L.; Scharf, D. A computer simulation of H10A24, a synthetic 4-helix bundle that binds halothane. *Toxicol. Lett.* **1998**, *101*, 377–385.
402. Tuckerman, M. E.; Mundy, C. J.; Balasubramanian, S.; Klein, M. L. Response to a comment on “Modified nonequilibrium molecular dynamics for fluid flows with energy conservation”. *J. Chem. Phys.* **1998**, *108*, 4353–4354.
403. Tuckerman, M. E.; Klein, M. L. Ab initio molecular dynamics of solid nitromethane. *Chem. Phys. Lett.* **1998**, *283*, 147–151.
404. Bandyopadhyay, S.; Klein, M. L.; Martyna, G. J.; Tarek, M. Molecular dynamics studies of the hexagonal mesophase of sodium dodecylsulphate in aqueous solution. *Mol. Phys.* **1998**, *95*, 377–384.
405. Tu, K.; Tarek, M.; Klein, M. L.; Scharf, D. Effects of anesthetics on the structure of a phospholipid bilayer: Molecular dynamics investigation of halothane in the hydrated liquid crystal phase of dipalmitoylphosphatidylcholine. *Biophys. J.* **1998**, *75*, 2123–2134.
406. Husslein, T.; Newns, D. M.; Pattnaik, P. C.; Zhong, Q.; Moore, P. B.; Klein, M. L. Constant pressure and temperature molecular-dynamics simulation of the hydrated diphytanolphosphatidylcholine lipid bilayer. *J. Chem. Phys.* **1998**, *109*, 2826–2832.
407. Miura, S.; Tuckerman, M. E.; Klein, M. L. An ab initio path integral molecular dynamics study of double proton transfer in the formic acid dimer. *J. Chem. Phys.* **1998**, *109*, 5290–5299.



408. Kinugawa, K.; Moore, P. B.; Klein, M. L. Centroid path integral molecular dynamics simulation of para-hydrogen slabs with lithium impurities. *J. Chem. Phys.* **1998**, *109*, 610–617.
409. Bandyopadhyay, S.; Tarek, M.; Klein, M. L. Computer simulation of amphiphilic interfaces. *Curr. Opin. Colloid Interface Sci.* **1998**, *3*, 242–246.
410. Tuckerman, M. E.; Mundy, C. J.; Klein, M. L. Response to a comment on “Toward a statistical thermodynamics of steady states”. *Phys. Rev. Lett.* **1998**, *80*, 4105–4106.
411. Tobias, D.; Tu, K.; Klein, M. L. Constant-pressure molecular dynamics investigation of cholesterol effects in a dipalmitoylphosphatidylcholine bilayer. *Biophys. J.* **1998**, *75*, 2147–2156.
412. Moore, P. B.; Zhong, Q.; Husslein, T.; Klein, M. L. Simulation of the HIV-1 Vpu transmembrane domain as a pentameric bundle. *FEBS Lett.* **1998**, *431*, 143–146.
413. Zhong, Q.; Husslein, T.; Newns, D.; Klein, M. L. Molecular dynamics simulations of the influenza A Virus M2 ion channel in a membrane-mimetic environment. *FEBS Lett.* **1998**, *434*, 265–271.
414. Mei, H. S.; Sagnella, D. E.; Klein, M. L.; Tuckerman, M. E. Quantum nuclear ab initio molecular dynamics study of water wires. *J. Phys. Chem. B* **1998**, *102*, 10446–10458.
415. Bandyopadhyay, S.; Shelley, J. C.; Tarek, M.; Klein, M. L. Surfactant aggregation at a hydrophobic surface. *J. Phys. Chem. B* **1998**, *102*, 6318–6322.
416. Balasubramanian, S.; Mundy, C. J.; Klein, M. L. Trimethylaluminum: Computer simulation studies of condensed phases and the gas-phase dimer. *J. Phys. Chem. B* **1998**, *102*, 10136–10141.
417. Diekmann, G. R.; Lear, J. D.; Zhong, Q.; Klein, M. L.; DeGrado, W. F.; Sharp, K. A. Exploration of the structural features defining the conduction properties of a synthetic ion channel. *Biophys. J.* **1999**, *76*, 618–630.
418. Saitta, A. M.; Soper, P. D.; Wasserman, E.; Klein, M. L. Influence of a knot on the strength of a polymer strand. *Nature* **1999**, *399*, 46–48.
419. Sprik, M.; Röthlisberger, U.; Klein, M. L. Conformational and orientational order and disorder in solid poly(tetrafluoroethylene). *Mol. Phys.* **1999**, *97*, 355–373.
420. Husslein, T.; Moore, P. B.; Zhong, Q.; Newns, D.; Pattnak, P.; Klein, M. L. Molecular dynamics simulation of a hydrated DiPhyPC lipid bilayer containing an alpha-helical bundle of four transmembrane domains of the influenza a virus M2 protein. *Faraday Discuss.* **1998**, *111*, 201–208.
421. Bandyopadhyay, S.; Tarek, M.; Klein, M. L. Computer simulation studies of surfactant systems. In *New Approaches to Problems in Liquid State Theory*; Caccamo, C., Hansen, J.-P., Stell, G., Eds.; NATO Science Series, Series C, Mathematical and Physical Sciences 529; Kluwer: Boston, MA, 1999; pp 347–354.
422. Bagchi, K.; Sullivan, D. M.; Tuckerman, M. E.; Klein, M. L. Ab initio molecular dynamics study of crystalline nitric acid trihydrates. *J. Phys. Chem. A* **1999**, *103*, 8678–8683.
423. Tarek, M.; Tu, K.; Klein, M. L.; Tobias, D. J. Molecular dynamics simulations of supported phospholipid/alkanethiol bilayers on a gold (111) surface. *Biophys. J.* **1999**, *77*, 964–972.
424. Saitta, A. M.; Klein, M. L. Evolution of fragments formed at the rupture of a knotted alkane molecule. *J. Am. Chem. Soc.* **1999**, *121*, 11827–11830.
425. Saitta, A. M.; Klein, M. L. Polyethylene under tensile load: Strain energy storage and breaking of linear and knotted alkanes probed by first principles molecular dynamics calculations. *J. Chem. Phys.* **1999**, *111*, 9434–9440.
426. Kim, D.; Klein, M. L. Ab initio molecular dynamics study of (HF)<sub>n</sub>BF<sub>3</sub> clusters. *Chem. Phys. Lett.* **1999**, *308*, 235–241.
427. Davies, L. A.; Klein, M. L.; Scharf, D. Molecular dynamics simulation of a synthetic four- $\alpha$ -helix bundle that binds the anesthetic halothane. *FEBS Lett.* **1999**, *455*, 332–338.
428. Bandyopadhyay, S.; Tarek, M.; Klein, M. L. Molecular dynamics study of lipid–DNA complexes. *J. Phys. Chem. B* **1999**, *103*, 10075–10080.
429. Bandyopadhyay, S.; Tarek, M.; Lynch, M.; Klein, M. L. Molecular dynamics study of the poly(oxyethylene) surfactant C<sub>12</sub>E<sub>2</sub> and water. *Langmuir* **2000**, *16*, 942–946.
430. Kim, D.; Klein, M. L. Liquid hydrogen fluoride with an excess proton: Ab initio molecular dynamics study of a superacid. *J. Am. Chem. Soc.* **1999**, *121*, 11251–11252.
431. Koubi, L.; Tarek, M.; Klein, M. L.; Scharf, D. Distribution of halothane in a DPPC bilayer from molecular dynamics calculations. *Biophys. J.* **2000**, *78*, 800–811.
432. Saitta, A. M.; Klein, M. L. First principles study of limiting stress and bond rupture of entangled polymer chains. *J. Phys. Chem. B* **2000**, *104*, 2197–2200.
433. Zhong, Q.; Newns, D.; Pattnak, P.; Lear, J. D.; Klein, M. L. Two possible conducting states of the M2 ion channel formed by the influenza a virus. *FEBS Lett.* **2000**, *473*, 195–198.
434. Yarne, D.; Tuckerman, M. E.; Klein, M. L. Structural and dynamical behavior of an azide ion in water from ab initio molecular dynamics calculations. *Chem. Phys.* **2000**, *258*, 163–169.
435. Mundy, C. J.; Balasubramanian, S.; Bagchi, K.; Tuckerman, M. E.; Martyna, G. J.; Klein, M. L. Non-equilibrium molecular dynamics. In *Reviews in Computational Chemistry*; Lipkowitz, K. B., Boyd, D. B., Eds.; Wiley: New York, 2000; Vol. 14, pp 291–397.
436. Davies, L. A.; Zhong, Q.; Klein, M. L.; Scharf, D. Molecular dynamics simulation of four- $\alpha$ -helix bundles that bind the anesthetic halothane. *FEBS Lett.* **2000**, *478*, 61–66.
437. Allen, R.; Bandyopadhyay, S.; Klein, M. L. C<sub>12</sub>E<sub>2</sub> reverse micelle: A molecular dynamics study. *Langmuir* **2000**, *16*, 10547–10552.
438. Kim, D.; Klein, M. L. Ab initio molecular dynamics study of the superacid system HF/SbF<sub>5</sub> solution. *J. Phys. Chem. B* **2000**, *104*, 10074–10079.
439. Newns, D. M.; Zhong, Q. F.; Moore, P. B.; Husslein, T.; Pattnaik, P.; Klein, M. L. Molecular dynamics study of structure and gating of low molecular weight ion channels. *Parallel Comput.* **2000**, *26*, 965–976.
440. Okada, O.; Klein, M. L. Phase transition and water molecules in titanylphthalocyanine phase Y crystal. *Phys. Chem. Chem. Phys.* **2001**, *3*, 1530–1534.

441. Lynch, M. L.; Wireko, F.; Tarek, M.; Klein, M. L. Intermolecular interactions and the structure of fatty acid-soap crystals. *J. Phys. Chem. B* **2001**, *105*, 552–561.
442. Klein, M. L. Water on the move. *Science* **2001**, *291*, 2106–2107.
443. Saiz, L.; Klein, M. L. Structural properties of highly polyunsaturated lipid bilayer from molecular dynamics simulations. *Biophys. J.* **2001**, *81*, 204–216.
444. Bandyopadhyay, S.; Shelley, J. C.; Klein, M. L. Molecular dynamics study of the effect of surfactant on a biomembrane. *J. Phys. Chem. B* **2001**, *105*, 5979–5986.
445. Shelley, J. C.; Shelley, M. Y.; Reeder, R. C.; Bandyopadhyay, S.; Klein, M. L. A coarse grained model for biomembrane simulations. *J. Phys. Chem. B* **2001**, *105*, 4464–4470.
446. Saitta, A. M.; Klein, M. L. First principles molecular dynamics study of the rupture processes of a bulk-like polyethylene knot. *J. Phys. Chem. B* **2001**, *105*, 6495–6499.
447. Raugei, S.; Klein, M. L. Ab Initio molecular dynamics investigation of the formyl cation in the superacid  $\text{SbF}_5/\text{HF}$ . *J. Phys. Chem. B* **2001**, *105*, 8212–8219.
448. Saiz, L.; Klein, M. L. Influence of highly polyunsaturated lipid acyl chains of biomembranes on the nmr order parameters. *J. Am. Chem. Soc.* **2001**, *123*, 7381–7387.
449. Moore, P. B.; Lopez, C.; Klein, M. L. Dynamical properties of a hydrated lipid bilayer from a multianosecond molecular dynamics simulation. *Biophys. J.* **2001**, *81*, 2484–2494.
450. Shelley, J. C.; Shelley, M. Y.; Reeder, R. C.; Bandyopadhyay, S.; Moore, P. B.; Klein, M. L. Simulations of phospholipids using a coarse grained model. *J. Phys. Chem. B* **2001**, *105*, 9785–9792.
451. Koubi, L.; Tarek, M.; Bandyopadhyay, S.; Klein, M. L.; Scharf, D. Membrane structural perturbations caused by anesthetics and non-immobilizers: A molecular dynamics study. *Biophys. J.* **2001**, *81*, 3339–3345.
452. Chen, B.; Siepmann, J. I.; Klein, M. L. Direct Gibbs ensemble Monte Carlo simulations for solid-vapor phase equilibria: Applications to Lennard-Jonesium and carbon dioxide. *J. Phys. Chem. B* **2001**, *105*, 9840–9848.
453. Tarek, M.; Tobias, D. J.; Chen, S. H.; Klein, M. L. Short wavelength collective dynamics in phospholipid bilayers: A molecular dynamics study. *Phys. Rev. Lett.* **2001**, *87*, 238101.
454. Raugei, S.; Klein, M. L. Dynamics of water molecules in the  $\text{Br}^-$  solvation shell: An ab initio molecular dynamics study. *J. Am. Chem. Soc.* **2001**, *123*, 9484–9485.
455. Chen, B.; Siepmann, J. I.; Oh, K.-J.; Klein, M. L. Aggregation-volume-bias Monte Carlo simulations of vapor-liquid nucleation barriers for Lennard-Jonesium. *J. Chem. Phys.* **2001**, *115*, 10903–10913.
456. Snyder, R. G.; Tu, K.; Klein, M. L.; Mendelssohn, R.; Strauss, H. L.; Sun, W. Acyl chain conformation and packing in dipalmitoylphosphatidylcholine bilayers from MD simulation and IR spectroscopy. *J. Phys. Chem. B* **2002**, *106*, 6273–6288.
457. Lopez, C. F.; Moore, P. B.; Shelley, J. C.; Shelley, M. Y.; Klein, M. L. Computer simulation of biomembranes using a coarse-grain model. *Comput. Phys. Commun.* **2002**, *147*, 1–6.
458. Lopez, C.; Montal, M.; Blasie, J. K.; Klein, M. L.; Moore, P. B. Molecular Dynamics investigation of membrane-bound bundles of the channel forming transmembrane domain of the viral protein U from the human immunodeficiency virus HIV-1. *Biophys. J.* **2002**, *83*, 1259–1267.
459. Saiz, L.; Klein, M. L. Electrostatic interactions in a neutral model phospholipid bilayer with highly unsaturated alkyl chains by molecular dynamics simulations. *J. Chem. Phys.* **2002**, *116*, 3052–3057.
460. Raugei, S.; Klein, M. L. An ab initio study of water molecules in the bromide ion solvation shell. *J. Chem. Phys.* **2002**, *116*, 196–202.
461. Saitta, A. M.; Klein, M. L. Molecular dynamics study of the influence of a knot on the stretching-induced crystallization of a polymer. *J. Chem. Phys.* **2002**, *116*, 5333–5336.
462. Tew, G.; Liu, D.; Chen, B.; Doerksen, R.; Kaplan, J.; Carroll, P. J.; Klein, M. L.; DeGrado, W. F. De novo design of biomimetic antimicrobial polymers. *Proc. Natl. Acad. Sci. U.S.A.* **2002**, *99*, 5110–5114.
463. Nordgren, C. E.; Tobias, D. J.; Klein, M. L.; Blasie, J. K. MD Simulation of a hydrated protein vectorially-oriented on polar and nonpolar soft surfaces. *Biophys. J.* **2002**, *83*, 2906–2917.
464. Chen, B.; Siepmann, J. I.; Oh, K.-J.; Klein, M. L. Simulating vapor-liquid nucleation in *n*-alkanes. *J. Chem. Phys.* **2002**, *116*, 4317–4329.
465. Saiz, L.; Bandyopadhyay, S.; Klein, M. L. Towards an understanding of complex biological membranes by atomistic molecular dynamics simulations. *Biosci. Rep.* **2002**, *22*, 151–174.
466. Raugei, S.; Klein, M. L. Structure of the strongly associated liquid antimony pentafluoride: An ab initio molecular dynamics study. *J. Chem. Phys.* **2002**, *116*, 7087–7093.
467. Chen, B.; Park, J. M.; Ivanov, I.; Tabacci, G.; Klein, M. L.; Parrinello, M. First principles study of aqueous hydroxide solutions. *J. Am. Chem. Soc.* **2002**, *124*, 8534–8535.
468. Saiz, L.; Klein, M. L. Computer simulation studies of model biological membranes. *Acc. Chem. Res.* **2002**, *35*, 482–489.
469. Raugei, S.; Klein, M. L. Application of density functional theory based Car-Parrinello simulations to the study of catalytic processes. *Quant. Struct.-Act. Relat.* **2002**, *22*, 149–165.
470. Koubi, L.; Scharf, D.; Klein, M. L. Distribution of non-immobilizer HFE in a model membrane. *Anesthesia* **2002**, *97*, 848–855.
471. Lopez, C. F.; Nielsen, S. O.; Moore, P. B.; Shelley, J. C.; Klein, M. L. Self-assembly of a Langmuir monolayer using coarse-grained molecular dynamics simulations. *J. Phys.: Condens. Matter* **2002**, *14*, 9431–9444.
472. Sillanpaa, A. J.; Simon, C.; Laasonen, K. E.; Klein, M. L. Structural and spectral properties of aqueous HF solutions using ab initio molecular dynamics. *J. Phys. Chem. B* **2002**, *106*, 11315–11322.
473. Raugei, S.; Klein, M. L. Hydrocarbon reactivity in the superacid  $\text{Sb}_5/\text{HF}$ : An ab initio molecular dynamics study. *J. Phys. Chem. B* **2002**, *106*, 11596–11605.

474. Chen, B.; Ivanov, I.; Park, J. M.; Parrinello, M.; Klein, M. L. Solvation structure and mobility mechanism of OH<sup>-</sup>: A Car–Parrinello molecular dynamics investigation of alkaline solutions. *J. Phys. Chem. B* **2002**, *106*, 12006–12016.
475. Chen, B.; Sipemmann, J. I.; Oh, K.-J.; Klein, M. L. Simulating vapor–liquid nucleation of *n*-alkanes. *J. Chem. Phys.* **2002**, *116*, 4317–4329.
476. Ivanov, I.; Klein, M. L. Histidine protonation in aqueous solution via constrained Car–Parrinello molecular dynamics. *J. Am. Chem. Soc.* **2002**, *124*, 13380–13381.
477. Nielsen, S. O.; Klein, M. L. A coarse grain model for lipid monolayers and bilayer studies. In *Bridging the Time Scales: Molecular Simulations for the Next Decade*; Nielabs, P., Maraschel, M., Ciccotti, G., Eds.; Springer: Berlin, 2002; pp 27–63.
478. Saitta, A. M.; Klein, M. L. Proton tunneling in fatty acid/soap crystals? *J. Chem. Phys.* **2003**, *118*, 1–3.
479. Papoyan, G.; DeGrado, W. F.; Klein, M. L. Probing the configurational space of a metalloprotein core: An ab initio molecular dynamics study of duo ferro 1 binuclear Zn cofactor. *J. Am. Chem. Soc.* **2003**, *125*, 560–569.
480. Chen, B.; Siepmann, J. I.; Klein, M. L. Simulating the nucleation of water/ethanol and water/*n*-nonane mixtures: mutual enhancement and two-pathway nucleation. *J. Am. Chem. Soc.* **2003**, *125*, 3113–3118.
481. Doerksen, R. J.; Chen, B.; Liu, D.; DeGrado, W. F.; Klein, M. L. Designed intramolecular hydrogen bonds stabilizing antimicrobial amphiphilic polymers. *Polym. Prepr.* **2003**, *44*, 598.
482. Magistrato, A.; DeGrado, W. F.; Laio, A.; Rothlisberger, U.; Vande Vondele, J.; Klein, M. L. Characterization of the dizinc analogue of the synthetic diiron protein df1 using ab initio and hybrid quantum/classical molecular dynamics simulations. *J. Phys. Chem. B* **2003**, *107*, 4182–4188.
483. Raugei, S.; Klein, M. L. Nuclear quantum effects and hydrogen bonding in liquids. *J. Am. Chem. Soc.* **2003**, *125*, 8992–8993.
484. Doerksen, R. J.; Chen, B.; Klein, M. L. Intramolecular hydrogen bonds: Ab initio Car–Parrinello simulations of arylamide torsions. *Chem. Phys. Lett.* **2003**, *380*, 150–157.
485. Nielsen, S. O.; Lopez, C. F.; Srinivas, G.; Klein, M. L. A coarse grain model for *n*-alkanes parameterized from surface tension data. *J. Chem. Phys.* **2003**, *119*, 7043–7049.
486. Yuan, J.; Chen, B.; Doerksen, R. J.; Klein, M. L.; Winkler, J. D. Novel conformationally-constrained  $\beta$ -peptides characterized by <sup>1</sup>H NMR chemical shifts. *Chem. Commun.* **2003**, *20*, 2534–2535.
487. Chen, B.; Ivanov, I.; Klein, M. L.; Parrinello, M. Hydrogen bonding in water. *Phys. Rev. Lett.* **2003**, *91*, 215503.
488. Nielsen, S. O.; Lopez, C. F.; Moore, P. B.; Shelley, J. C.; Klein, M. L. Molecular dynamics investigations of lipid Langmuir monolayers using a coarse grain model. *J. Phys. Chem. B* **2003**, *107*, 13911–13917.
489. Koubi, L.; Saiz, L.; Tarek, M.; Scharf, D.; Klein, M. L. Influence of anesthetic and nonimmobilizer molecules on the physical properties of a polyunsaturated lipid bilayer. *J. Phys. Chem. B* **2003**, *107*, 14500–14508.
490. Ivanov, I.; Klein, M. L. First principles computational study of the active site of arginase. *Proteins: Struct., Funct., Genet.* **2004**, *54*, 1–7.
491. Pophristic, V.; Klein, M. L.; Holerca, M. N. Modeling of small aluminum chlorohydrate polymers. *J. Phys. Chem. A* **2004**, *108*, 113–120.
492. Saiz, L.; Bandyopadhyay, S.; Klein, M. L. Effect of a pore region of a transmembrane ion channel on the physical properties of a simple membrane. *J. Phys. Chem. B* **2004**, *107*, 2608–2613.
493. Liu, D.; Choi, S.; Chen, B.; Doerksen, R. R.; Clements, D. J.; Winkler, J. D.; Klein, M. L.; DeGrado, W. F. Nontoxic membrane-active antimicrobial arylamide oligomers. *Angew. Chem., Int. Ed.* **2004**, *44*, 1158–1162.
494. Lopez, C. F.; Nielsen, S. O.; Moore, P. B.; Klein, M. L. Understanding nature's design for a nanosyringe. *Proc. Natl. Acad. Sci. U.S.A.* **2004**, *101*, 4431–4434.
495. Kuo, J.-L.; Klein, M. L. Dissociation of hydrogen fluoride in HF(H<sub>2</sub>O)<sub>7</sub>. *J. Chem. Phys.* **2004**, *120*, 4690–4695.
496. Kim, E.-G.; Klein, M. L. Unknotting of a polymer strand in a melt. *Macromolecules* **2004**, *37*, 1674–1677.
497. Pophristic, V.; Klein, M. L.; Balagurusamy, V. S. K. Structure and dynamics of Al<sub>13</sub>O<sub>4</sub>(OH)<sub>24</sub>(H<sub>2</sub>O)<sub>12</sub>C<sub>17</sub> polymer. *Phys. Chem. Chem. Phys.* **2004**, *6*, 919–923.
498. Nielsen, S. O.; Lopez, C. F.; Srinivas, G.; Klein, M. L. Coarse grain models and the computer simulation of soft materials. *J. Phys.: Condens. Matter* **2004**, *16*, R481–R512.
499. Nielsen, S. O.; Lopez, C. F.; Moore, P. B.; Klein, M. L. Hydrogen bonding structure and dynamics of water at the DMPC lipid bilayer surface from a molecular dynamics simulation. *J. Phys. Chem. B* **2004**, *108*, 6603–6610.
500. Nielsen, S. O.; Lopez, C. F.; Ivanov, I.; Moore, P. B.; Shelley, J. C.; Klein, M. L. Transmembrane peptide induced lipid sorting and mechanism of the L $\alpha$  to inverted phase transition using coarse grain molecular dynamics. *Biophys. J.* **2004**, *87*, 2107–2115.
501. Srinivas, G.; Lopez, C. F.; Klein, M. L. Membrane-bound hydrophiles facilitate cation translocation. *J. Phys. Chem. B* **2004**, *108*, 4231–4235.
502. Kim, E.-G.; Klein, M. L. Density functional study of ethylene–norbornene copolymerization via metallocene and constrained-geometry catalysts. *Organometallics* **2004**, *23*, 3319–3326.
503. Srinivas, G.; Shelley, J. C.; Nielsen, S. O.; Discher, D. E.; Klein, M. L. Simulation of diblock copolymer self-assembly using a coarse-grain model. *J. Phys. Chem. B* **2004**, *108*, 8153–8160.
504. Srinivas, G.; Discher, D. E.; Klein, M. L. Self-assembly and properties of diblock copolymers by coarse-grain molecular dynamics. *Nat. Mater.* **2004**, *3*, 638–644.
505. Srinivas, G.; Klein, M. L. Computational approaches to nanobiotechnology: Probing the interaction of synthetic molecules with phospholipid bilayers via a coarse grain model. *Nanotechnology* **2004**, *15*, 1289–1295.
506. Ensing, B.; Laio, A.; Gervasio, F. L.; Parrinello, M.; Klein, M. L. A minimum free energy reaction path for the E2 reaction between fluoro ethane and a fluoride ion. *J. Am. Chem. Soc.* **2004**, *126*, 9492–9493.
507. Feng, I.; Kuo, W.; Mundy, C. J.; McGrath, M. J.; Siepmann, J. I.; Vandevondele, J.; Sprik, M.; Hutter, J.; Chen, B.; Klein, M. L.; Mohamed, F.; Krack, M.; Parrinello, M. Liquid water from first principles: Investigation of different sampling approaches. *J. Phys. Chem. B* **2004**, *108*, 12990–12998.



508. Srinivas, G.; Klein, M. L. Coarse-grain molecular dynamics simulations of diblock copolymer surfactants interacting with a lipid bilayer. *Mol. Phys.* **2004**, *102*, 883–890.
509. Kuo, J.-L.; Klein, M. L. Structure of ice-VII and ice-VIII: A quantum mechanical study. *J. Phys. Chem. B* **2004**, *108*, 19634–19639.
510. Raugei, S.; Klein, M. L. On the quantum nature of an excess proton in liquid hydrogen fluoride. *ChemPhysChem* **2004**, *5*, 1569–1576.
511. Doerksen, R. J.; Chen, B.; Liu, D.; Tew, G. N.; DeGrado, W. F.; Klein, M. L. Controlling the conformation of arylamides: Computational studies of intramolecular hydrogen bonds between amides and ethers or thioethers. *Chem.—Eur. J.* **2004**, *10*, 5008–5016.
512. Kuo, J. L.; Klein, M. L.; Kuhs, W. F. The effect of proton disorder on the structure of ice-Ih: A theoretical study. *J. Chem. Phys.* **2005**, *123*, 134505.
513. Lin, C.-K.; Wu, C.-C.; Wang, Y.-S.; Lee, Y. T.; Chang, H.-C.; Kuo, J.-L.; Klein, M. L. Vibrational predissociation spectra and hydrogen-bond topologies of  $\text{H}^+(\text{H}_2\text{O})_{9-11}$ . *Phys. Chem. Chem. Phys.* **2005**, *7*, 938–944.
514. Saiz, L.; Klein, M. L. The transmembrane domain of the acetylcholine receptor: Insights from simulations on synthetic peptide models. *Biophys. J.* **2005**, *88*, 959–970.
515. Pickholz, M.; Saiz, L.; Klein, M. L. Concentration effects of volatile anesthetics on the properties of model membrane: A coarse grain approach. *Biophys. J.* **2005**, *88*, 1524–1534.
516. Simon, C.; Klein, M. L. Ab initio molecular dynamics simulation of a water–hydrogen fluoride equimolar mixture. *ChemPhysChem* **2005**, *6*, 148–153.
517. Chen, B.; Siepmann, J. I.; Klein, M. L. Simulating vapor–liquid nucleation of water: A combined histogram-reweighting and aggregation-volume-bias Monte Carlo investigation for fixed-charge and polarizable models. *J. Phys. Chem. A* **2005**, *109*, 1137–1145.
518. Mella, M.; Kuo, J. L.; Clary, D. C.; Klein, M. L. Nuclear quantum effects on the structure and energetics of  $(\text{H}_2\text{O})_6\text{H}^+$ . *Phys. Chem. Chem. Phys.* **2005**, *7*, 2324–2332.
519. Dal Peraro, M.; Raugei, S.; Carloni, P.; Klein, M. L. Solute–solvent charge transfer in aqueous solution. *ChemPhysChem* **2005**, *6*, 1715–1718.
520. Kuo, J. L.; Klein, M. L. Structure of protonated water clusters: Low-energy structures and finite temperature. *J. Chem. Phys.* **2005**, *122*, 024516.
521. Ensing, B.; Laio, A.; Parrinello, M.; Klein, M. L. A recipe for the computation of the free energy barrier and lowest free energy path of concerted reactions. *J. Phys. Chem. B* **2005**, *109*, 6676–6687.
522. Lopez, C. F.; Nielsen, S. O.; Ensing, B.; Moore, P. B.; Klein, M. L. Structure and dynamics of model pore insertion into a membrane. *Biophys. J.* **2005**, *88*, 3083–3094.
523. Ivanov, I.; Klein, M. L. Dynamical flexibility and proton transfer in the arginase active site probed by ab initio molecular dynamics. *J. Am. Chem. Soc.* **2005**, *127*, 4010–4020.
524. Ensing, B.; Klein, M. L. Perspective on the reactions between  $\text{F}^-$  and  $\text{CH}_3\text{CH}_2\text{F}$ : The free energy landscape of the E2 and  $\text{S}_{\text{N}}2$  reaction channels. *Proc. Natl. Acad. Sci. U.S.A.* **2005**, *102*, 6755–6759.
525. Chang, H.-C.; Jiang, J.-C.; Kuo, J.-L.; Klein, M. L. Protonated clathrate cages enclosing neutral water molecules:  $\text{H}^+(\text{H}_2\text{O})_{21}$  and  $\text{H}^+(\text{H}_2\text{O})_{28}$ . *J. Chem. Phys.* **2005**, *122*, 74315.
526. Singer, S. J.; Kuo, J.-L.; Hirsch, T. K.; Knight, C.; Ojamae, L.; Klein, M. L. Hydrogen bond topology and the ice VII/VIII and Ih/XI proton ordering phase transitions. *Phys. Rev. Lett.* **2005**, *94*, 135701.
527. Nielsen, S. O.; Ensing, B.; Ortiz, V.; Moore, P. B.; Klein, M. L. Lipid bilayer perturbations around a transmembrane nanotube: A coarse grain molecular dynamics study. *Biophys. J.* **2005**, *88*, 3822–3828.
528. DeVivo, M.; Ensing, B.; Klein, M. L. Computational study of phosphatase activity in soluble epoxide hydrolase: High efficiency through a water bridge mediated proton shuttle. *J. Am. Chem. Soc.* **2005**, *127*, 11226–11227.
529. Nielsen, S. O.; Srinivas, G.; Lopez, C. F.; Klein, M. L. Modeling surfactant adsorption in solid surfaces. *Phys. Rev. Lett.* **2005**, *94*, 228301.
530. Nielsen, S. O.; Srinivas, G.; Klein, M. L. Incorporating a hydrophobic solid into a coarse-grain liquids framework: Graphite in an aqueous amphiphilic environment. *J. Chem. Phys.* **2005**, *123*, 124907.
531. Ortiz, V.; Nielsen, S. O.; Klein, M. L.; Discher, D. E. Unfolding a linker between helical repeats. *J. Mol. Biol.* **2005**, *349*, 638–647.
532. Choi, S.; Clements, D. J.; Pophristic, V.; Ivanov, I.; Vempavala, S.; Bennett, J. S.; Klein, M. L.; Winkler, J. D.; DeGrado, W. F. The design and evaluation of heparin-binding foldamers. *Angew. Chem., Int. Ed.* **2005**, *44*, 6685–6689.
533. Ortiz, V.; Nielsen, S. O.; Discher, D. E.; Klein, M. L.; Shillcock, J.; Lipowsky, R. Dissipative particle dynamics simulations of polymersomes. *J. Phys. Chem. B* **2005**, *109*, 17708–17714.
534. Srinivas, G.; Discher, D. E.; Klein, M. L. Key roles for chain flexibility in block copolymer membranes that contain pores or make tubes. *Nano Lett.* **2005**, *5*, 2343–2349.
535. Domene, C.; Vempavala, S.; Klein, M. L.; Vénien-Bryan, C.; Doyle, D. A. Role of aromatic localization in the gating process of a potassium channel. *Biophys. J.* **2006**, *90*, L1–L3.