

List of publications

Michele Parrinello

Articles

1. "Itinerant theory of ferromagnetism and Hund's-rule coupling"
T. Arai and M. Parrinello
Phys. Rev. Lett. **27**, 1226 (1971)
2. "Electron correlations and plasmon dispersion in metals"
M. Parrinello and M. P. Tosi
Nuovo Cim. **12B**, 155 (1972)
3. "Electron-ion triplet correlations in liquid metals"
M. Parrinello and M. P. Tosi
J. Phys. C **6**, L254 (1973)
4. "Perturbation expansion of the antiferromagnetic ground state"
M. Parrinello, M. Scirè and T. Arai
Lett. Nuovo Cim. **6**, 138 (1973)
5. "Optical modes in binary alloys"
M. C. Abramo, M. Parrinello, M. P. Tosi and D. E. Thornton
Phys. Lett. **43A**, 483 (1973)
6. "Correlations in ionic melts I. Static structure factors and dielectric properties"
M. C. Abramo, M. Parrinello and M. P. Tosi
J. Nonmetals **2**, 57 (1973)
7. "Correlations in ionic melts II. Moments of current correlations"
M. C. Abramo, M. Parrinello and M. P. Tosi
J. Nonmetals **2**, 67 (1974)
8. "Dynamic structure factors and neutron scattering in molten salts"
M. C. Abramo, M. Parrinello and M. P. Tosi
J. Phys. C **7**, 4201 (1974)
9. "Infinite-order cumulant expansion for spins"
M. Parrinello and T. Arai
Phys. Rev. B **10**, 265 (1974)
10. "Electronic effects in dynamical structure of liquid metals"
M. P. Tosi, M. Parrinello and N. H. March
Nuovo Cim. **23B**, 135 (1974)

11. "Partial structure factors and atomic dynamics in conformal solutions"
M. Parrinello, M. P. Tosi and N. H. March
Proc. R. Soc. London A **341**, 91 (1974)
12. "Concentration dependence of electrical transport coefficients in conformal liquid metal alloys"
M. Parrinello, N. H. March and M. P. Tosi
J. Phys. F **4**, L142 (1974)
13. "On the susceptibility sum rule in the electron liquid"
C. Caccamo, G. Pizzimenti, M. Parrinello and M. P. Tosi
Lett. Nuovo Cim. **11**, 156 (1974)
14. "Excitations and atomic transport in classical binary isotopic fluids"
M. Parrinello, M. P. Tosi and N. H. March
J. Phys. C **7**, 2577 (1974)
15. "Mass and charge transport in a simple molten salt"
P. V. Giaquinta, M. Parrinello and M. P. Tosi
J. Phys. C **8**, L501 (1975)
16. "Dynamical correlations in the one-component plasma"
M. C. Abramo and M. Parrinello
Lett. Nuovo Cim. **12**, 667 (1975)
17. "Is the Haeffner effect in liquid metals related to the electrical resistivity of the isotopic mixture?"
M. Parrinello, M. P. Tosi and N. H. March
Lett. Nuovo Cim. **12**, 605 (1975)
18. "Wavenumber-dependent concentration fluctuations in liquid mixtures"
M. W. Johnson, N. H. March, D. I. Page, M. Parrinello and M. P. Tosi
J. Phys. C **8**, 751 (1975)
19. "Concentration dependence of partial structure factors in liquid mixtures"
M. Parrinello and M. P. Tosi
Nuovo Cim. **25B**, 242 (1975)
20. "Thermodynamics of Wigner crystallization"
M. Parrinello and N. H. March
J. Phys. C **9**, L147 (1976)
21. "Structure factors of liquids containing chemical complexes"
N. H. March, M. Parrinello and M. P. Tosi
Phys. Chem. Liq. **5**, 39 (1976)
22. "Radius-ratio effects in the structure of fluids of charged hard spheres"
M. C. Abramo, C. Caccamo, G. Pizzimenti, M. Parrinello and M. P. Tosi
J. Phys. C **9**, L593 (1976)

23. "Electron-electron pair correlation function in solid and molten nearly-free electron metals"
S. Cusack, N. H. March, M. Parrinello and M. P. Tosi
J. Phys. F **6**, 749 (1976)
24. "Hydrodynamic correlation functions for molten salts"
P. V. Giaquinta, M. Parrinello and M. P. Tosi
Phys. Chem. Liq. **5**, 305 (1976)
25. "Frequency spectra of transport properties in ionic liquids: contribution of charge fluctuation modes"
P. V. Giaquinta, M. Parrinello, M. P. Tosi and N. H. March
Phys. Chem. Liq. **5**, 197 (1976)
26. "Plasmons and excitons in insulators: dielectric treatment"
P. V. Giaquinta, M. Parrinello, E. Tosatti and M. P. Tosi
J. Phys. C **9**, 2031 (1976)
27. "Plasmon bands and gaps in metal crystals"
R. Girlanda, M. Parrinello and E. Tosatti
Phys. Rev. Lett. **36**, 1386 (1976)
28. "Diffusion and structure of nickel chloride in aqueous solution"
R. Mills, N. H. March, P. V. Giaquinta, M. Parrinello and M. P. Tosi
Chem. Phys. **26**, 237 (1977)
29. "Photoelectron spectroscopy and hole-electron valence bound state in crystalline xenon"
M. Parrinello, E. Tosatti, N. H. March and M. P. Tosi
Lett. Nuovo Cim. **18**, 341 (1977)
30. "Electrical resistivity of liquid rare-earth metals"
M. Parrinello, N. H. March and M. P. Tosi
Nuovo Cim. **39B**, 233 (1977)
31. "Charge fluctuation spectra at very long wave-length in ionic fluids"
P. V. Giaquinta, M. Parrinello, W. Bouché and M. P. Tosi
Lett. Nuovo Cim. **19**, 215 (1977)
32. "Linear specific heat of disordered solids at low temperatures"
P. V. Giaquinta, N. H. March, M. Parrinello and M. P. Tosi
Phys. Rev. Lett. **39**, 41 (1977)
33. "Polaritonic spectra of ionic conductors"
P. V. Giaquinta, M. Parrinello and M. P. Tosi
J. Phys. C **11**, 4821 (1978)
34. "Ionic radii and diffraction patterns of molten alkali halides"
M. C. Abramo, C. Caccamo, G. Pizzimenti, M. Parrinello and M. P. Tosi
J. Chem. Phys. **68**, 2889 (1978)

35. “Optical absorption of dilute solutions of metals in molten salts”
G. Senatore, M. Parrinello and M. P. Tosi
Lett. Nuovo Cim. **23**, 629 (1978)
36. “Collective dynamics of charge fluctuations in ionic conductors”
P. V. Giaquinta, M. Parrinello and M. P. Tosi
Physica **92A**, 185 (1978)
37. “Dynamic density fluctuations in molten salts: diagonalized-relaxation theory for liquid RbBr”
M. C. Abramo, M. Parrinello and M. P. Tosi
Phys. Chem. Liq. **8**, 1 (1978)
38. “Static dielectric behavior of charged fluids near freezing”
A. Fasolino, M. Parrinello and M. P. Tosi
Phys. Lett. **66A**, 119 (1978)
39. “Phenomenological theory of first- and second-order metal-insulator transitions at absolute zero”
N. H. March, M. Suzuki and M. Parrinello
Phys. Rev. B **19**, 2027 (1979)
40. “Analytic solution of the mean spherical approximation for a multi-component plasma”
M. Parrinello and M. P. Tosi
Chem. Phys. Lett. **64**, 579 (1979)
41. “Small-angle scattering from molten salts”
M. Rovere, P. V. Giaquinta, M. Parrinello and M. P. Tosi
Phil. Mag. B **39**, 167 (1979)
42. “Gas-liquid transition in charged fluids”
M. Rovere, R. Miniero, M. Parrinello and M. P. Tosi
Phys. Chem. Liq. **9**, 11 (1979)
43. “Crystal structure and pair potentials: a molecular-dynamics study”
M. Parrinello and A. Rahman
Phys. Rev. Lett. **45**, 1196 (1980)
44. “Partial structure factors in molten alkali halide mixtures”
M. C. Abramo, C. Caccamo, G. Pizzimenti and M. Parrinello
Mol. Phys. **40**, 1421 (1980)
45. “Optical absorption of dilute solutions of metals in molten salts”
G. Senatore, M. Parrinello and M. P. Tosi
Phil. Mag. B **41**, 595 (1980)
46. “Structure and thermodynamics of two-component classical plasmas in the mean spherical approximation”
G. Senatore, M. Rovere, M. Parrinello and M. P. Tosi
Nuovo Cim. **56B**, 39 (1980)

47. "Polymorphic transitions in single crystals: a new molecular dynamics method"
M. Parrinello and A. Rahman
J. Appl. Phys. **52**, 7182 (1981), DOI: 10.1063/1.328693
48. "Analytical solution of a new integral equation for triplet correlations in hard sphere fluids"
M. Parrinello and P. V. Giaquinta
J. Chem. Phys. **74**, 1990 (1981)
49. "Polymorphic transitions in alkali halides. A molecular dynamics study"
M. Parrinello and A. Rahman
J. de Phys. **42**, C6-511 (1981)
50. "Strain fluctuations and elastic constants"
M. Parrinello and A. Rahman
J. Chem. Phys. **76**, 2662 (1982)
51. "Molecular phases in a lattice-gas model"
M. Parrinello and E. Tosatti
Phys. Rev. Lett. **49**, 1165 (1982)
52. "Outline of a theory of the two-dimensional Hall effect in the quantum limit"
E. Tosatti and M. Parrinello
Lett. Nuovo Cim. **36**, 289 (1983)
53. "Pair correlations near a hard wall: an analytical theory"
P. V. Giaquinta and M. Parrinello
J. Chem. Phys. **78**, 1946 (1983)
54. "Structural transitions in superionic conductors"
M. Parrinello, A. Rahman and P. Vashishta
Phys. Rev. Lett. **50**, 1073 (1983)
55. "Pair correlations at an electrified interface"
P. V. Giaquinta and M. Parrinello
J. Chem. Phys. **81**, 4074 (1984)
56. "Coexistence of atomic and molecular phases in a two-dimensional lattice-gas model"
G. M. Florio, P. V. Giaquinta, M. Parrinello and E. Tosatti
Phys. Rev. Lett. **52**, 1899 (1984)
57. "Monte Carlo study of the phase diagram of a two-dimensional system of hard cyclic hexamers"
K. W. Wojciechowski, A. Brańka and M. Parrinello
Mol. Phys. **53**, 1541 (1984)
58. "Study of an *F* center in molten KCl"
M. Parrinello and A. Rahman
J. Chem. Phys. **80**, 860 (1984), DOI: 10.1063/1.446740

59. “Unified approach for molecular dynamics and density-functional theory”
R. Car and M. Parrinello
Phys. Rev. Lett. **55**, 2471 (1985)
60. “Free energy evaluation in the canonical molecular dynamics ensemble”
A. Brańka and M. Parrinello
Mol. Phys. **58**, 989 (1986)
61. “Au(100) surface reconstruction”
F. Ercolessi, E. Tosatti and M. Parrinello
Phys. Rev. Lett. **57**, 719 (1986)
62. “Au(100) reconstruction in the glue model”
F. Ercolessi, M. Parrinello and E. Tosatti
Surf. Sci. **177**, 314 (1986)
63. “Free energy of formation of lattice vacancies in silicon”
G. B. Bachelet, G. Jacucci, R. Car and M. Parrinello
18th Int. Conf. Phys. Semicond., Stockholm, Sweden, 11-15 August 1986, **2**, 801. Editor(s):
Engstrom, O. Publisher: World Scientific, Singapore (1987)
64. “Electron pairing in dilute liquid metal-metal halide solutions”
A. Selloni, R. Car, M. Parrinello and P. Carnevali
J. Phys. Chem. **91**, 4947 (1987)
65. “Polaron theory of electrons solvated in molten salts”
G. Malescio and M. Parrinello
Phys. Rev. A **35**, 897 (1987)
66. “Localization, hopping, and diffusion of electrons in molten salts”
A. Selloni, P. Carnevali, R. Car and M. Parrinello
Phys. Rev. Lett. **59**, 823 (1987)
67. “Temperature-dependent phonons of the c(2x2) reconstructed W(001) surface”
C. Z. Wang, E. Tosatti, A. Fasolino and M. Parrinello
Surf. Sci. **189/190**, 679 (1987)
68. “Au surface reconstructions in the glue model”
F. Ercolessi, A. Bartolini, M. Garofalo, M. Parrinello and E. Tosatti
Surf. Sci. **189/190**, 636 (1987)
69. “The structure of selenium clusters - Se₃ to Se₈”
D. Hohl, R. O. Jones, R. Car and M. Parrinello
Chem. Phys. Lett. **139**, 540 (1987)
70. “Molecular dynamics studies of gold surfaces”
F. Ercolessi, A. Bartolini, M. Garofalo, M. Parrinello and E. Tosatti
Phys. Scr. **T19**, 399 (1987)

71. “The unified approach to density functional and molecular dynamics in real space”
R. Car and M. Parrinello
Solid State Comm. **62**, 403 (1987)
72. “Structure of sulfur clusters using simulated annealing: S₂ to S₁₃”
D. Hohl, R. O. Jones, R. Car and M. Parrinello
J. Chem. Phys. **89**, 6823 (1988)
73. “Bipolarons in metal-metal halide solutions”
E. S. Fois, A. Selloni, M. Parrinello and R. Car
J. Phys. Chem. **92**, 3268 (1988)
74. “Equilibrium structures and finite temperature properties of silicon microclusters from *ab initio* molecular-dynamics calculations”
P. Ballone, W. Andreoni, R. Car and M. Parrinello
Phys. Rev. Lett. **60**, 271 (1988)
75. “Simulation of gold in the glue model”
F. Ercolessi, M. Parrinello and E. Tosatti
Phil. Mag. A **58**, 213 (1988)
76. “Structural, dynamical, and electronic properties of amorphous silicon: an *ab initio* molecular-dynamics study”
R. Car and M. Parrinello
Phys. Rev. Lett. **60**, 204 (1988)
77. “Reconstruction phase transition of the clean W(001) surface”
C. Z. Wang, M. Parrinello, E. Tosatti and A. Fasolino
Europhys. Lett. **6**, 43 (1988)
78. “Numerical simulation of the 1D and 2D Hubbard models: Fermi liquid behavior and its breakdown”
S. Sorella, E. Tosatti, S. Baroni, R. Car and M. Parrinello
Int. J. Mod. Phys. B **2**, 993 (1988)
79. “Simulation of electrons in molten salts”
A. Selloni, E. S. Fois, M. Parrinello and R. Car
Phys. Scr. **T25**, 261 (1989)
80. “Approach to metallic behavior in metal-molten-salt solutions”
E. Fois, A. Selloni and M. Parrinello
Phys. Rev. B **39**, 4812 (1989)
81. “Bonding and disorder in liquid silicon”
I. Štich, R. Car and M. Parrinello
Phys. Rev. Lett. **63**, 2240 (1989)
82. “Carbon: the nature of the liquid state”
G. Galli, R. M. Martin, R. Car and M. Parrinello
Phys. Rev. Lett. **63**, 988 (1989)

83. "Energy surfaces and structure of S₇O"
D. Hohl, R. O. Jones, R. Car and M. Parrinello
J. Am. Chem. Soc. **111**, 825 (1989)
84. "A novel technique for the simulation of interacting fermion systems"
S. Sorella, S. Baroni, R. Car and M. Parrinello
Europhys. Lett. **8**, 663 (1989)
85. "Structural and electronic properties of amorphous carbon"
G. Galli, R. M. Martin, R. Car and M. Parrinello
Phys. Rev. Lett. **62**, 555 (1989)
86. "Proton diffusion in crystalline silicon"
F. Buda, G. L. Chiarotti, R. Car and M. Parrinello
Phys. Rev. Lett. **63**, 294 (1989)
87. "Conjugate gradient minimization of the energy functional: a new method for electronic structure calculation"
I. Štich, R. Car, M. Parrinello and S. Baroni
Phys. Rev. B **39**, 4997 (1989)
88. "Numerical study of the 2D Hubbard model at half filling"
S. Sorella, A. Parola, M. Parrinello and E. Tosatti
Int. J. Mod. Phys. B **3**, 1875 (1989)
89. "Temperature and segregation effects in alkali-metal microclusters from *ab initio* molecular dynamics simulations"
P. Ballone, W. Andreoni, R. Car and M. Parrinello
Europhys. Lett. **8**, 73 (1989)
90. "Dipolar atoms, spin-paired species and the anomalous behavior of Na-NaBr solutions"
L. F. Xu, A. Selloni and M. Parrinello
Chem. Phys. Lett. **162**, 27 (1989)
91. "Recent numerical results on the two dimensional Hubbard model"
A. Parola, S. Sorella, S. Baroni, R. Car, M. Parrinello and E. Tosatti
Physica C **162-164**, 771 (1989)
92. "Ab-initio molecular-dynamics of liquid and amorphous semiconductors"
F. Buda, G. L. Chiarotti, I. Štich, R. Car and M. Parrinello
J. Non-Cryst. Solids **114**, 7 (1989)
93. "First-principles molecular dynamics simulations of disordered materials"
R. Car and M. Parrinello
Europhys. News **20**, 69 (1989)
94. "Static properties of the 2D Hubbard model on a 4x4 cluster"
A. Parola, S. Sorella, S. Baroni, M. Parrinello and E. Tosatti
Int. J. Mod. Phys. B **3**, 1865 (1989)

95. "Liquid arsenic: comparison of *ab initio* and pair-potential predictions of molecular structure"
X. P. Li, P. B. Allen, R. Car, M. Parrinello and J. Q. Broughton
Phys. Rev. B **41**, 3260 (1990)
96. "Atomic structure and bonding in liquid GaAs"
Q. M. Zhang, G. Chiarotti, A. Selloni, R. Car and M. Parrinello
J. Non-Cryst. Solids **117/118**, 930 (1990)
97. "Atomic structure and bonding in liquid GaAs from *ab initio* molecular dynamics"
Q. M. Zhang, G. Chiarotti, A. Selloni, R. Car and M. Parrinello
Phys. Rev. B **42**, 5071 (1990)
98. "Melting of diamond at high pressure"
G. Galli, R. M. Martin, R. Car and M. Parrinello
Science **250**, 1547 (1990)
99. "Thermal expansion of *c*-Si via *ab initio* molecular dynamics"
F. Buda, R. Car and M. Parrinello
Phys. Rev. B **41**, 1680 (1990)
100. "Non-Fermi-liquid exponents of the one-dimensional Hubbard model"
S. Sorella, A. Parola, M. Parrinello and E. Tosatti
Europhys. Lett. **12**, 721 (1990)
101. "Structural, electronic, and vibrational properties of Si(111)-2x1 from *ab initio* molecular dynamics"
F. Ancilotto, W. Andreoni, A. Selloni, R. Car and M. Parrinello
Phys. Rev. Lett. **65**, 3148 (1990)
102. "*Ab initio* molecular dynamics simulation of molten KSi"
G. Galli and M. Parrinello
J. Phys.: Condens. Matter **2**, SA227 (1990)
103. "*Ab initio* calculation of properties of carbon in the amorphous and liquid states"
G. Galli, R. M. Martin, R. Car and M. Parrinello
Phys. Rev. B **42**, 7470 (1990)
104. "Dipolar atoms and spin paired species in Na-NaBr solutions"
L. F. Xu, A. Selloni and M. Parrinello
J. Non-Cryst. Solids **117/118**, 926 (1990)
105. "Hydrogen in crystalline and amorphous silicon. A first principles molecular dynamics study"
F. Buda, G. L. Chiarotti, R. Car and M. Parrinello
Physica B **119**, 98 (1991)
106. "Theoretical study of LiC₆"
J. Kohanoff, G. Galli and M. Parrinello
J. de Phys. IV **1**, C5-351 (1991)

107. "Surface phonons and dipole activity of Si(111)2x1 from *ab initio* calculations"
F. Ancilotto, A. Selloni, W. Andreoni, S. Baroni, R. Car and M. Parrinello
Phys. Rev. B **43**, 8930 (1991)
108. " α -gallium: a metallic molecular crystal"
X. G. Gong, G. L. Chiarotti, M. Parrinello and E. Tosatti
Phys. Rev. B **43**, 14277 (1991)
109. "*d*-wave, dimer, and chiral states in the two-dimensional Hubbard model"
A. Parola, S. Sorella, M. Parrinello and E. Tosatti
Phys. Rev. B **43**, 6190 (1991)
110. "Structure of hydrogenated amorphous silicon from *ab initio* molecular dynamics"
F. Buda, G. L. Chiarotti, R. Car and M. Parrinello
Phys. Rev. B **44**, 5908 (1991)
111. "Electronic and vibrational properties of C₆₀ at finite temperature from *ab initio* molecular dynamics"
B. P. Feuston, W. Andreoni, M. Parrinello and E. Clementi
Phys. Rev. B **44**, 4056 (1991)
112. "Theoretical study of molten KSi"
G. Galli and M. Parrinello
J. Chem. Phys. **95**, 7504 (1991)
113. "Amorphous silicon studied by *ab initio* molecular dynamics: preparation, structure, and properties"
I. Štich, R. Car and M. Parrinello
Phys. Rev. B **44**, 11092 (1991)
114. "Structural, bonding, dynamical, and electronic properties of liquid silicon: an *ab initio* molecular-dynamics study"
I. Štich, R. Car and M. Parrinello
Phys. Rev. B **44**, 4262 (1991)
115. "Comment on 'Error cancellation in the molecular dynamics method for total energy calculations'"
R. Car, M. Parrinello and M. Payne
J. Phys.: Condens. Matter **3**, 9539 (1991)
116. "Structural properties of amorphous SiC via *ab-initio* molecular dynamics"
F. Finocchi, G. Galli, M. Parrinello and M. Bertoni
J. Non-Cryst. Solids, **137-138**, 153 (1991)
117. "Structural and electronic properties of C₇₀"
W. Andreoni, F. Gygi and M. Parrinello
Chem. Phys. Lett. **189**, 241 (1992)
118. "Doping-induced distortions and bonding in K₆C₆₀ and Rb₆C₆₀"
W. Andreoni, F. Gygi and M. Parrinello
Phys. Rev. Lett. **68**, 823 (1992)

119. "Impurity states in doped fullerenes: C₅₉B and C₅₉N"
W. Andreoni, F. Gygi and M. Parrinello
Chem. Phys. Lett. **190**, 159 (1992)
120. Microscopic structure of amorphous covalent alloys probed by *ab initio* molecular dynamics: SiC"
F. Finocchi, G. Galli, M. Parrinello and C. M. Bertoni
Phys. Rev. Lett. **68**, 3044 (1992)
121. "Adiabaticity in first-principles molecular dynamics"
P. E. Blöchl and M. Parrinello
Phys. Rev. B **45**, 9413 (1992)
122. "Alkali adsorption on Si(111) surfaces: *ab initio* molecular dynamics studies"
I. Moullet, W. Andreoni and M. Parrinello
Surf. Sci. **269-270**, 1000 (1992)
123. "Water dimer properties in the gradient-corrected density functional theory"
K. Laasonen, F. Csajka and M. Parrinello
Chem. Phys. Lett. **194**, 172 (1992)
124. "Si(111):Na: structural and electronic properties from *ab initio* molecular dynamics"
I. Moullet, W. Andreoni and M. Parrinello
Phys. Rev. B **46**, 1842 (1992)
125. "*Ab initio* studies on high pressure phases of ice"
C. Lee, D. Vanderbilt, K. Laasonen, R. Car and M. Parrinello
Phys. Rev. Lett. **69**, 462 (1992)
126. "Optical properties of porous silicon: a first-principles study"
F. Buda, J. Kohanoff and M. Parrinello
Phys. Rev. Lett. **69**, 1272 (1992)
127. "Zero-point-motion effects on the structure of C₆₀"
J. Kohanoff, W. Andreoni and M. Parrinello
Phys. Rev. B **46**, 4371 (1992)
128. "A possible new highly stable fulleride cluster: Li₁₂ C₆₀"
J. Kohanoff, W. Andreoni and M. Parrinello
Chem. Phys. Lett. **198**, 472 (1992)
129. "Reconstruction of the diamond (111) surface"
S. Iarlori, G. Galli, F. Gygi, M. Parrinello and E. Tosatti
Phys. Rev. Lett. **69**, 2947 (1992)
130. "Large scale electronic structure calculations"
G. Galli and M. Parrinello
Phys. Rev. Lett. **69**, 3547 (1992)

131. "Structural and electronic properties of La@C₈₂"
K. Laasonen, W. Andreoni and M. Parrinello
Science **258**, 1916 (1992)
132. "Intermolecular interactions and the nature of orientational ordering in the solid fullerenes C₆₀ and C₇₀"
A. Cheng, M. Klein, M. Parrinello and M. Sprik
Phil. Trans. R. Soc. Lond. A **341**, 327 (1992)
133. "First principles molecular dynamics: A modern tool for theoretical modeling of molecules and materials"
W. Andreoni, R. Car, M. Parrinello and A. Selloni
Chemical Design Automation News, 7, 1 (1992)
134. "Ab initio studies on the structural and dynamical properties of ice"
C. Lee, D. Vanderbilt, K. Laasonen, R. Car and M. Parrinello
Phys. Rev. B **47**, 4863 (1993)
135. "Structures of small water clusters using gradient-corrected density functional theory"
K. Laasonen, M. Parrinello, R. Car, C. Lee and D. Vanderbilt
Chem. Phys. Lett. **207**, 208 (1993)
136. "Ab initio liquid water"
K. Laasonen, M. Sprik, M. Parrinello and R. Car
J. Chem. Phys. **99**, 9080 (1993)
137. "Chemical order in amorphous covalent alloys: a theoretical study of a-SiC"
F. Finocchi, G. Galli, M. Parrinello and C. M. Bertoni
Physica B **185**, 379 (1993)
138. "Coexistence of monatomic and diatomic molecular fluid character in liquid gallium"
X. G. Gong, G. L. Chiarotti, M. Parrinello and E. Tosatti
Europhys. Lett. **21**, 469 (1993)
139. "Structure of nanoscale silicon clusters"
U. Röthlisberger, W. Andreoni and M. Parrinello
Phys. Rev. Lett. **72**, 665 (1994)
140. "Absence of metal clusters and appearance of new electron states in Na₆C₆₀"
W. Andreoni, P. Giannozzi and M. Parrinello
Phys. Rev. Lett. **72**, 848 (1994)
141. "Ab initio molecular dynamics of C₇₀. Intramolecular vibrations and zero-point motion effects"
G. Onida, W. Andreoni, J. Kohanoff and M. Parrinello
Chem. Phys. Lett. **219**, 1 (1994)
142. "Structural phase transformations via first-principles simulation"
P. Focher, G. L. Chiarotti, M. Bernasconi, E. Tosatti and M. Parrinello
Europhys. Lett. **26**, 345 (1994)

143. “*Ab initio* simulations of water and water ions”
M. E. Tuckerman, K. Laasonen, M. Sprik and M. Parrinello
J. Phys. Condens. Matter **6**, A93 (1994)
144. “Properties of supercritical water: an *ab initio* simulation”
E. S. Fois, M. Sprik and M. Parrinello
Chem. Phys. Lett. **223**, 411 (1994)
145. “Hydrolysis at stepped MgO surfaces”
W. Langel and M. Parrinello
Phys. Rev. Lett. **73**, 504 (1994)
146. “*Ab initio* path-integral molecular dynamics”
D. Marx and M. Parrinello
Z. Physik B **95**, 143 (1994)
147. “Integrating the Car-Parrinello equations. I. Basic integration techniques”
M. E. Tuckerman and M. Parrinello
J. Chem. Phys. **101**, 1302 (1994)
148. “Integrating the Car-Parrinello equations. II. Multiple time scale techniques”
M. E. Tuckerman and M. Parrinello
J. Chem. Phys. **101**, 1316 (1994)
149. “‘*Ab initio*’ liquid water and the conductive state of the excess electron”
K. Laasonen, M. Sprik and M. Parrinello
AIP Conf. Proc. **298** (Ultrafast Reaction Dynamics and Solvent Effects), 87 (1994)
150. “Exponential transformation of molecular orbitals”
J. Hutter, M. Parrinello and S. Vogel
J. Chem. Phys. **101**, 3862 (1994)
151. “*Ab initio* molecular dynamics with excited electrons”
A. Alavi, J. Kohanoff, M. Parrinello and D. Frenkel
Phys. Rev. Lett. **73**, 2599 (1994)
152. “Density-functional-theory-based molecular dynamics study of 1,3,5-trioxane and 1,3-dioxolane protolysis”
A. Curioni, W. Andreoni, J. Hutter, H. Schiffer and M. Parrinello
J. Am. Chem. Soc. **116**, 11251 (1994)
153. “Nature of the conduction states in the metallic molecular crystal $\text{Li}(\text{NH}_3)_4$ ”
J. Kohanoff, F. Buda, M. Parrinello and M. L. Klein
Phys. Rev. Lett. **73**, 3133 (1994)
154. “Electronic and geometric structure of $\text{La}@\text{C}_{82}$ and C_{82} : theory and experiment”
D. M. Poirier, M. Knupfer, J. H. Weaver, W. Andreoni, K. Laasonen, M. Parrinello, D. S. Bethune, K. Kikuchi and Y. Achiba
Phys. Rev. B **49**, 17403 (1994)

155. "Molecular structure and chemical bonding in K_3C_{60} and K_6C_{60} "
W. Andreoni, P. Giannozzi and M. Parrinello
Phys. Rev. B **51**, 2087 (1995)
156. "Structure and bonding in cisplatin and other Pt(II) complexes"
P. Carloni, W. Andreoni, J. Hutter, A. Curioni, P. Giannozzi and M. Parrinello
Chem. Phys. Lett. **234**, 50 (1995)
157. "Electronic structure of the Cu, Zn superoxide dismutase active site and its interactions with the substrate"
P. Carloni, P. E. Blöchl and M. Parrinello
J. Phys. Chem. **99**, 1338 (1995)
158. "Density functional study of small aqueous Be^{2+} clusters"
D. Marx, J. Hutter and M. Parrinello
Chem. Phys. Lett. **241**, 457 (1995)
159. "First-principle-constant pressure molecular dynamics"
M. Bernasconi, G. L. Chiarotti, P. Focher, S. Scandolo, E. Tosatti and M. Parrinello
J. Phys. Chem. Solids **56**, 501 (1995)
160. "*Ab initio* molecular dynamics simulation of the solvation and transport of H_3O^+ and OH^- ions in water"
M. Tuckerman, K. Laasonen, M. Sprik and M. Parrinello
J. Phys. Chem. **99**, 5749 (1995)
161. "*Ab initio* molecular dynamics of H_2O adsorbed on solid MgO "
W. Langel and M. Parrinello
J. Chem. Phys. **103**, 3240 (1995)
162. "Integrating the Car-Parrinello equations. III. Techniques for ultrasoft pseudopotentials"
J. Hutter, M. Tuckerman and M. Parrinello
J. Chem. Phys. **102**, 859 (1995)
163. "Structural quantum effects and three-centre two-electron bonding in CH_5^+ "
D. Marx and M. Parrinello
Nature **375**, 216 (1995)
164. "First principles investigation of quinizarin chemisorbed on $\alpha-Al_2O_3$ "
I. Frank, D. Marx and M. Parrinello
J. Am. Chem. Soc. **117**, 8037 (1995)
165. "*Ab initio* molecular dynamics simulation of the solvation and transport of hydronium and hydroxyl ions in water"
M. Tuckerman, K. Laasonen, M. Sprik and M. Parrinello
J. Chem. Phys. **103**, 150 (1995)
166. "Carboplatin versus cisplatin: density functional approach to their molecular properties"
E. Tornaghi, W. Andreoni, P. Carloni, J. Hutter and M. Parrinello
Chem. Phys. Lett. **246**, 469 (1995)

167. "Ab initio calculation of the sound velocity of dense hydrogen: implications for models of Jupiter"
A. Alavi, M. Parrinello and D. Frenkel
Science **269**, 1252 (1995)
168. "Static and dynamic density functional investigation of hydrated beryllium dications"
D. Marx, E. S. Fois and M. Parrinello
Int. J. Quant. Chem. **57**, 655 (1996)
169. "The effect of quantum and thermal fluctuations on the structure of the floppy molecule $C_2H_3^+$ "
D. Marx and M. Parrinello
Science **271**, 179 (1996)
170. "Response function basis sets: application to density functional calculations"
G. Lippert, J. Hutter, P. Ballone and M. Parrinello
J. Phys. Chem. **100**, 6231 (1996)
171. "Nonmetal-metal transition in metal-molten-salt solutions"
P. L. Silvestrelli, A. Alavi, M. Parrinello and D. Frenkel
Phys. Rev. B **53**, 12750 (1996)
172. "Hot electrons and the approach to metallic behaviour in $K_x(KCl)_{1-x}$ "
P. L. Silvestrelli, A. Alavi, M. Parrinello and D. Frenkel
Europhys. Lett. **33**, 551 (1996)
173. "New high-pressure phase of ice"
M. Benoit, M. Bernasconi, P. Focher and M. Parrinello
Phys. Rev. Lett. **76**, 2934 (1996)
174. "Geometry and electronic structure of porphyrins and porphyrazines"
D. Lamoen and M. Parrinello
Chem. Phys. Lett. **248**, 309 (1996)
175. "Efficient and general algorithms for path integral Car-Parrinello molecular dynamics"
M. E. Tuckerman, D. Marx, M. L. Klein and M. Parrinello
J. Chem. Phys. **104**, 5579 (1996)
176. "Ab initio path integral molecular dynamics: Basic ideas"
D. Marx and M. Parrinello
J. Chem. Phys. **104**, 4077 (1996)
177. "Microscopic structure of tetrahedral amorphous carbon"
N. A. Marks, D. R. McKenzie, B. A. Pailthorpe, M. Bernasconi and M. Parrinello
Phys. Rev. Lett. **76**, 768 (1996)
178. "Ab initio simulations of tetrahedral amorphous carbon"
N. A. Marks, D. R. McKenzie, B. A. Pailthorpe, M. Bernasconi and M. Parrinello
Phys. Rev. B **54**, 9703 (1996)

179. "Anisotropic α -C:H from compression of polyacetylene"
M. Bernasconi, M. Parrinello, G. L. Chiarotti, P. Focher and E. Tosatti
Phys. Rev. Lett. **76**, 2081 (1996)
180. "Structure and electronic properties of quinizarin chemisorbed on alumina"
I. Frank, D. Marx and M. Parrinello
J. Chem. Phys. **104**, 8143 (1996)
181. "*Ab initio* molecular dynamics simulation of liquid water: comparison of three gradient-corrected density functionals"
M. Sprik, J. Hutter and M. Parrinello
J. Chem. Phys. **105**, 1142 (1996)
182. "Nonempirical calculations of a hydrated RNA duplex"
J. Hutter, P. Carloni and M. Parrinello
J. Am. Chem. Soc. **118**, 8710 (1996)
183. "*Ab initio* molecular dynamics simulation of laser melting of silicon"
P. L. Silvestrelli, A. Alavi, M. Parrinello and D. Frenkel
Phys. Rev. Lett. **77**, 3149 (1996)
184. "Electronic structure, screening, and charging effects at a metal/organic tunneling junction: a first-principles study"
D. Lamoen, P. Ballone and M. Parrinello
Phys. Rev. B **54**, 5097 (1996)
185. "Response function basis sets: application to density functional calculations"
G. Lippert, J. Hutter, P. Ballone and M. Parrinello
J. Phys. Chem. **100**, 6231 (1996)
186. "Ionic diffusion in a ternary superionic conductor: an *ab initio* molecular dynamics study"
S. Wengert, R. Nesper, W. Andreoni and M. Parrinello
Phys. Rev. Lett. **77**, 5083 (1996)
187. "A *first principles* investigation of the structure of a bacteriochlorophyll crystal"
M. Marchi, J. Hutter and M. Parrinello
J. Am. Chem. Soc. **118**, 7847 (1996)
188. "Dynamics, spin fluctuations, and bonding in liquid silicon"
I. Štich, M. Parrinello and J. M. Holender
Phys. Rev. Lett. **76**, 2077 (1996)
189. "Two dimensional ice adsorbed on mica surface"
M. Odelius, M. Bernasconi and M. Parrinello
Phys. Rev. Lett. **78**, 2855 (1997)
190. "*Ab initio* molecular dynamics simulation of liquid hydrogen fluoride"
U. R othlisberger and M. Parrinello
J. Chem. Phys. **106**, 4658 (1997)

191. "Density functional theory-based molecular dynamics simulation of acid-catalyzed chemical reactions in liquid trioxane"
A. Curioni, M. Sprik, W. Andreoni, H. Schiffer, J. Hutter and M. Parrinello
J. Am. Chem. Soc. **119**, 7218 (1997)
192. "On the quantum nature of the shared proton in hydrogen bonds"
M. E. Tuckerman, D. Marx, M. L. Klein and M. Parrinello
Science **275**, 817 (1997)
193. "Solid-state polymerization of acetylene under pressure: *ab initio* simulation"
M. Bernasconi, G. L. Chiarotti, P. Focher, M. Parrinello and E. Tosatti
Phys. Rev. Lett. **78**, 2008 (1997)
194. "A density functional study of iron-porphyrin complexes"
C. Rovira, P. Ballone and M. Parrinello
Chem. Phys. Lett. **271**, 247 (1997)
195. "Electrical-conductivity calculation in *ab initio* simulations of metals: application to liquid sodium"
P. L. Silvestrelli, A. Alavi and M. Parrinello
Phys. Rev. B **55**, 15515 (1997)
196. "Self-assembled peptide nanotubes from first principles"
P. Carloni, W. Andreoni and M. Parrinello
Phys. Rev. Lett. **79**, 761 (1997)
197. "Structural, dynamical, electronic, and bonding properties of laser-heated silicon: an *ab initio* molecular-dynamics study"
P. L. Silvestrelli, A. Alavi, M. Parrinello and D. Frenkel
Phys. Rev. B **56**, 3806 (1997)
198. "Condensed matter effects on the structure of crystalline glucose"
C. Molteni and M. Parrinello
Chem. Phys. Lett. **275**, 409 (1997)
199. "Proton-induced plasticity in hydrogen clusters"
I. Štich, D. Marx, M. Parrinello and K. Terakura
Phys. Rev. Lett. **78**, 3669 (1997)
200. "Ab initio infrared spectrum of liquid water"
P. L. Silvestrelli, M. Bernasconi and M. Parrinello
Chem. Phys. Lett. **277**, 478 (1997)
201. "Defect-defect interactions in ionic conductors: a classical MD and MC study"
F. Zimmer, P. Ballone, J. Maier and M. Parrinello
Ber. Bunsenges. Phys. Chem. **101**, 1333 (1997)
202. "Protonated hydrogen clusters"
I. Štich, D. Marx, M. Parrinello and K. Terakura
J. Chem. Phys. **107**, 9482 (1997)

203. "Interaction of alkene radical cations with solvent molecules as described with density functional theory"
M. Mohr, H. Zipse, D. Marx and M. Parrinello
J. Phys. Chem. A **101**, 8942 (1997)
204. "Ab initio molecular dynamics study of polyfluoride anions"
T. von Rosenvinge, M. Parrinello and M. L. Klein
J. Chem. Phys. **107**, 8012 (1997)
205. "Infrared absorption in amorphous silicon from ab initio molecular dynamics"
A. Debernardi, M. Bernasconi, M. Cardona and M. Parrinello
Appl. Phys. Lett. **71**, 2692 (1997)
206. "A hybrid Gaussian and plane wave density functional scheme"
G. Lippert, J. Hutter and M. Parrinello
Mol. Phys. **92**, 477 (1997)
207. "Structure and dynamics of protonated Mg₂SiO₄: an ab-initio molecular dynamics study"
M. Haiber, P. Ballone and M. Parrinello
Am. Mineral. **82**, 913 (1997)
208. "Ab initio molecular dynamics of ion solvation. The case of Be²⁺ in water"
D. Marx, M. Sprik and M. Parrinello
Chem. Phys. Lett. **273**, 360 (1997)
209. "Structure and dynamics of protonated methane: CH₅⁺ at finite temperatures"
D. Marx and M. Parrinello
Z. Phys. D **41**, 253 (1997)
210. "Equilibrium geometries and electronic structure of iron-porphyrin complexes: a density functional study"
C. Rovira, K. Kunc, J. Hutter, P. Ballone and M. Parrinello
J. Phys. Chem. A **101**, 8914 (1997)
211. "The dissociation mechanism of H₂O in water studied by first-principles molecular dynamics"
B. L. Trout and M. Parrinello
Chem. Phys. Lett. **288**, 343 (1998)
212. "First principles molecular dynamics study of Ziegler-Natta heterogeneous catalysis"
M. Boero, M. Parrinello and K. Terakura
J. Am. Chem. Soc. **120**, 2746 (1998)
213. "Tunnelling and zero-point motion in high-pressure ice"
M. Benoit, D. Marx and M. Parrinello
Nature **392**, 258 (1998)
214. "A comparative study of O₂, CO, and NO binding to iron-porphyrin"
C. Rovira, K. Kunc, J. Hutter, P. Ballone and M. Parrinello
J. Quant. Chem. **69**, 31 (1998)

215. "Molecular dynamics in low-spin excited states"
I. Frank, J. Hutter, D. Marx and M. Parrinello
J. Chem. Phys. **108**, 4060 (1998)
216. "*Ab initio* molecular dynamics simulation of laser melting of graphite"
P. L. Silvestrelli and M. Parrinello
J. Appl. Phys. **83**, 2478 (1998)
217. "Glucose in aqueous solution by first principles molecular dynamics"
C. Molteni and M. Parrinello
J. Am. Chem. Soc. **120**, 2168 (1998)
218. "*Ab initio* infrared absorption study of the hydrogen-bond symmetrization in ice"
M. Bernasconi, P. L. Silvestrelli and M. Parrinello
Phys. Rev. Lett. **81**, 1235 (1998)
219. "Maximally-localized Wannier functions for disordered systems: application to amorphous silicon"
P. L. Silvestrelli, N. Marzari, D. Vanderbilt and M. Parrinello
Sol. State Comm. **107**, 7 (1998)
220. "Grid-free DFT implementation of local and gradient-corrected XC functionals"
G. Berghold, J. Hutter and M. Parrinello
Theor. Chem. Acc. **99**, 344 (1998)
221. "Understanding the nature of water bound to solid acid surfaces. *Ab initio* simulation on HSAPO-34"
V. Termath, F. Haase, J. Sauer, J. Hutter and M. Parrinello
J. Am. Chem. Soc. **120**, 8512 (1998)
222. "Oxygen binding to iron-porphyrin: a density functional study using both LSD and LSD+GC schemes"
C. Rovira and M. Parrinello
Int. J. Quant. Chem. **70**, 387 (1998)
223. "Density-functional study of hydration of sodium in water clusters"
L. M. Ramaniah, M. Bernasconi and M. Parrinello
J. Chem. Phys. **109**, 6839 (1998)
224. "Insight into chemical reactions from first-principles simulations: the mechanism of the gas-phase reaction of OH radicals with ketones"
I. Frank, M. Parrinello and A. Klamt
J. Phys. Chem. A **102**, 3614 (1998)
225. "Pressure effects on hydrogen bonding in the disordered phase of solid HBr"
T. Ikeda, M. Sprik, K. Terakura and M. Parrinello
Phys. Rev. Lett. **81**, 4416 (1998)

226. "A hybrid method for solutes in complex solvents: Density functional theory combined with empirical force fields"
M. Eichinger, P. Tavan, J. Hutter and M. Parrinello
J. Chem. Phys. **110**, 10452 (1999)
227. "Ab initio study of structural and electronic properties of yttria-stabilized cubic zirconia"
G. Stapper, M. Bernasconi, N. Nicoloso and M. Parrinello
Phys. Rev. B **59**, 797 (1999)
228. "Superionic and metallic states of water and ammonia at giant planet conditions"
C. Cavazzoni, G. L. Chiarotti, S. Scandolo, E. Tosatti, M. Bernasconi and M. Parrinello
Science **283**, 44 (1999)
229. "The nature of the hydrated excess proton in water"
D. Marx, M. E. Tuckerman, J. Hutter and M. Parrinello
Nature **397**, 601 (1999)
230. "CH₅⁺: the Cheshire cat smiles"
D. Marx and M. Parrinello
Science **284**, 59 (1999)
231. "Factors influencing ligand-binding properties of heme models: a first principles study of picket-fence and protoheme complexes"
C. Rovira and M. Parrinello
Chem. Eur. J. **5**, 250 (1999)
232. "Pressure-induced structural changes of HBr"
T. Ikeda, M. Sprik, K. Terakura and M. Parrinello
Physica **B 265**, 101 (1999)
233. "Density-functional study of hydration of ammonium in water clusters"
F. Brugé, M. Bernasconi and M. Parrinello
J. Chem. Phys. **110**, 4734 (1999)
234. "Water molecule dipole in the gas and in the liquid phase"
P. L. Silvestrelli and M. Parrinello
Phys. Rev. Lett. **82**, 3308 (1999)
235. "Ab initio molecular-dynamics simulation of K⁺ solvation in water"
L. M. Ramaniah, M. Bernasconi and M. Parrinello
J. Chem. Phys. **111**, 1587 (1999)
236. "Pressure-induced structural and chemical changes of solid HBr"
T. Ikeda, M. Sprik, K. Terakura and M. Parrinello
J. Chem. Phys. **111**, 1595 (1999)
237. "Structural, electronic, and bonding properties of liquid water from first principles"
P. L. Silvestrelli and M. Parrinello
J. Chem. Phys. **111**, 3572 (1999)

238. "The iron-sulfur bond in cytochrome *c*"
C. Rovira, P. Carloni and M. Parrinello
J. Phys. Chem. B **103**, 7031 (1999)
239. "Static structure and dynamical correlations in high pressure H₂S"
R. Rousseau, M. Boero, M. Bernasconi, M. Parrinello and K. Terakura
Phys. Rev. Lett. **83**, 2218 (1999)
240. "Analysis of the dissociation of H₂O in water using first-principles molecular dynamics"
B. Trout and M. Parrinello
J. Phys. Chem. B **103**, 7340 (1999)
241. "First-principles molecular dynamics study of a photochromic molecular crystal"
I. Frank, D. Marx and M. Parrinello
J. Phys. Chem. A **103**, 7341 (1999)
242. "First principles calculations of Si doped fullerenes: structural and electronic localization properties in C₅₉Si and C₅₈Si₂"
I. M. L. Billas, C. Massobrio, M. Boero, M. Parrinello, W. Branz, F. Tast, N. Malinowski, M. Heinebrodt and T. P. Martin
J. Chem. Phys. **111**, 6787 (1999)
243. "CH₅⁺ stability and mass spectrometry. Comment by: George M. Kramer. Response by: T. Oka, E. White, D. Marx and M. Parrinello"
Science **286**, 1051a (1999)
244. "An excited state density functional theory study of the rhodopsin chromophore"
C. Molteni, I. Frank and M. Parrinello
J. Am. Chem. Soc. **121**, 12177 (1999)
245. "Ab initio simulation of rotational dynamics of solvated ammonium ion in water"
F. Brugé, M. Bernasconi and M. Parrinello
J. Am. Chem. Soc. **121**, 10883 (1999)
246. "The Gaussian and augmented-plane-wave density functional method for ab initio molecular dynamics simulations"
G. Lippert, J. Hutter and M. Parrinello
Theor. Chem. Acc. **103**, 124 (1999)
247. "Ab initio molecular dynamics with a classical pressure reservoir: simulation of pressure-induced amorphization in a Si₃₅H₃₆ cluster"
R. Martoňák, C. Molteni and M. Parrinello
Phys. Rev. Lett. **84**, 682 (2000)
248. "Harmonic and anharmonic dynamics of Fe-CO and Fe-O₂ in heme models"
C. Rovira and M. Parrinello
Biophys. J. **78**, 93 (2000)
249. "First principles study of propene polymerization in Ziegler-Natta heterogeneous catalysis"
M. Boero, M. Parrinello, S. Hüffer and H. Weiss
J. Am. Chem. Soc. **122**, 501 (2000)

250. "The conductivity anomaly in PbF_2 : a numerical investigation by classical MD and MC simulations"
F. Zimmer, P. Ballone, M. Parrinello and J. Maier
Solid State Ionics **127**, 277 (2000)
251. "Solvated excess protons in water: quantum effects on the hydration structure"
D. Marx, M. Tuckerman and M. Parrinello
J. Phys.: Condens. Matter **12**, A 153 (2000)
252. "A density functional theory study of a silica-supported zirconium monohydride catalyst for depolymerization of polyethylene"
J. J. Mortensen and M. Parrinello
J. Phys. Chem. B **104**, 2901 (2000)
253. "Charge carrier interactions in ionic conductors: a classical molecular-dynamics and Monte Carlo study on AgI"
F. Zimmer, P. Ballone, J. Maier and M. Parrinello
J. Chem. Phys. **112**, 6416 (2000)
254. "Two-membered silicon rings on the dehydroxylated surface of silica"
D. Ceresoli, M. Bernasconi, S. Iarlori, M. Parrinello and E. Tosatti
Phys. Rev. Lett. **84**, 3887 (2000)
255. "Ab initio analysis of proton transfer dynamics in $(\text{H}_2\text{O})_3\text{H}^+$ "
P. Geissler, C. Dellago, D. Chandler, J. Hutter and M. Parrinello
Chem. Phys. Lett. **321**, 225 (2000)
256. "All-electron *ab-initio* molecular dynamics"
M. Krack and M. Parrinello
Phys. Chem. Chem. Phys. **2**, 2105 (2000)
257. "General and efficient algorithms for obtaining maximally localized Wannier functions"
G. Berghold, C. J. Mundy, A. Romero, J. Hutter and M. Parrinello
Phys. Rev. B **61**, 10040 (2000)
258. "Density functional study of ^{17}O NMR chemical shift and nuclear quadrupole coupling tensors in oxyheme model complexes"
M. Kaupp, C. Rovira and M. Parrinello
J. Phys. Chem. B **104**, 5200 (2000)
259. "Microsolvation and chemical reactivity of sodium and water clusters"
C. J. Mundy, J. Hutter and M. Parrinello
J. Am. Chem. Soc. **122**, 4837 (2000)
260. "*Ab initio* simulation of phase transitions and dissociation of H_2S at high pressure"
R. Rousseau, M. Boero, M. Bernasconi, M. Parrinello and K. Terakura
Phys. Rev. Lett. **85**, 1254 (2000)

261. "Hydrogen bonding and dipole moment of water at supercritical conditions: a first-principles molecular dynamics study"
M. Boero, K. Terakura, T. Ikeshoji, C. C. Liew and M. Parrinello
Phys. Rev. Lett. **85**, 3245 (2000)
262. "Generalized variational density functional perturbation theory"
A. Putrino, D. Sebastiani and M. Parrinello
J. Chem. Phys. **113**, 7102 (2000)
263. "Solvation of radical cations in water – reactive or unreactive solvation?"
M. Mohr, D. Marx, M. Parrinello and H. Zipse
Chem. Eur. J. **6**, 4009 (2000)
264. "First-principles molecular dynamics simulations of models for the myoglobin active center"
C. Rovira and M. Parrinello
Int. J. Quant. Chem. **80**, 1172 (2000)
265. "Hydrogen elimination and solid-state reaction in hydrogen-bonded systems under pressure: the case of HBr"
T. Ikeda, M. Sprik, K. Terakura and M. Parrinello
J. Phys. Chem B **104**, 11801 (2000)
266. "First principles calculations of iron-doped heterofullerenes"
I. M. L. Billas, C. Massobrio, M. Boero, M. Parrinello, W. Branz, F. Tast, N. Malinowski, M. Heinebrodt and T. P. Martin
Comp. Mat. Science **17**, 191 (2000)
267. "A comparative study of galactose oxidase and active site analogs based on QM/MM Car-Parrinello simulations"
U. Röthlisberger, P. Carloni, K. Doclo and M. Parrinello
J. Biol. Inorg. Chem. **5**, 236 (2000)
268. "An anomalous alloy: Y_xSi_{1-x} "
V. Meregalli and M. Parrinello
Sol. State Comm. **117**, 441 (2001)
269. "First principles molecular dynamics simulations of pressure-induced structural transformations in silicon clusters"
C. Molteni, R. Martoňák and M. Parrinello
J. Chem. Phys. **114**, 5358 (2001)
270. "Surface solvation of halogen anions in water clusters: An *ab initio* molecular dynamics study of the $Cl^-(H_2O)_6$ complex"
D. J. Tobias, P. Jungwirth and M. Parrinello
J. Chem. Phys. **114**, 7036 (2001)
271. "Autoionization in liquid water"
P. L. Geissler, C. Dellago, D. Chandler, J. Hutter and M. Parrinello
Science **291**, 2121 (2001)

272. "Compton scattering and the character of the hydrogen bond in ice I_h "
A. Romero, P. L. Silvestrelli and M. Parrinello
J. Chem. Phys. **115**, 115 (2001)
273. "Structural and electronic properties of co-corrole, co-corrin, and co-porphyrin"
C. Rovira, K. Kunc, J. Hutter and M. Parrinello
Inorg. Chem. **40**, 11 (2001)
274. "A new ab-initio approach for NMR chemical shifts in periodic systems"
D. Sebastiani and M. Parrinello
J. Phys. Chem. A **105**, 1951 (2001)
275. "A first principles exploration of a variety of active surfaces and catalytic sites in Ziegler-Natta heterogeneous catalysis"
M. Boero, M. Parrinello, H. Weiss and S. Hüffer
J. Phys. Chem. A **105**, 5096 (2001)
276. "Water at supercritical conditions: a first principles study"
M. Boero, K. Terakura, T. Ikeshoji, C. C. Liew and M. Parrinello
J. Chem. Phys. **115**, 2219 (2001)
277. "Localized non-orthogonal orbitals in silicon"
J. J. Mortensen and M. Parrinello
J. Phys.: Condens. Matter **13**, 5731 (2001)
278. "Influence of the heme pocket conformation on the structure and vibrations of the Fe-CO bond in myoglobin: a QM/MM density functional study"
C. Rovira, B. Schulze, M. Eichinger, J. D. Evanseck and M. Parrinello
Biophys. J. **81**, 435 (2001)
279. "Vibrational analysis from linear response theory"
F. Filippone and M. Parrinello
Chem. Phys. Lett. **345**, 179 (2001)
280. "A novel implicit Newton-Raphson geometry optimization method for density functional theory calculations"
F. Filippone, S. Meloni and M. Parrinello
J. Chem. Phys. **115**, 636 (2001)
281. "Action-derived molecular dynamics in the study of rare events"
D. Passerone and M. Parrinello
Phys. Rev. Lett. **87**, 108302 (2001)
282. "Dehydroxylation and silanization of the surfaces of β -cristobalite silica: an ab initio simulation"
S. Iarlori, D. Ceresoli, M. Bernasconi, D. Donadio and M. Parrinello
J. Phys. Chem. B **105**, 8007 (2001)

283. "Ab initio molecular dynamics-based assignment of the protonation state of pepstatin A/HIV-1 protease cleavage site"
S. Piana, D. Sebastiani, P. Carloni and M. Parrinello
J. Am. Chem. Soc. **123**, 8730 (2001)
284. "Formation of a reactive intermediate in molecular beam chemistry of sodium and water"
F. Mercuri, C. J. Mundy and M. Parrinello
J. Phys. Chem. A **105**, 8423 (2001)
285. "Review of theoretical calculations of hydrogen storage in carbon-based materials"
V. Meregalli and M. Parrinello
Appl. Phys. A **72**, 143 (2001)
286. "Efficient $k \cdot p$ method for the calculation of total energy and electronic density of states"
M. Iannuzzi and M. Parrinello
Phys. Rev. B. **64**, 233104 (2001)
287. "Medium effects on ^{51}V NMR chemical shifts: a density functional study"
M. Bühl and M. Parrinello
Chem. Eur. J. **20**, 4487 (2001)
288. "Accurate total energies without self-consistency"
D. M. Benoit, D. Sebastiani and M. Parrinello
Phys. Rev. Lett. **87**, 226401 (2001)
289. "Interaction of short-chain alkane thiols and thiolates with small gold clusters: Adsorption structures and energetics"
D. Krüger, H. Fuchs, D. Marx and M. Parrinello
J. Chem. Phys. **115**, 4776 (2001)
290. "Polarized atomic orbitals for linear scaling methods"
G. Berghold, J. Hutter and M. Parrinello
J. Chem. Phys. **116**, 1800 (2002)
291. "Cesiumauride ammonia (1/1), $\text{CsAu} \cdot \text{NH}_3$: a crystalline analogue to alkali metals dissolved in ammonia?"
A.-V. Mudring, M. Jansen, J. Daniels, S. Krämer, M. Mehring, J. P. Prates Ramalho, A. H. Romero and M. Parrinello
Angew. Chem. Int. Ed. **41**, 120 (2002)
292. "Role of conformational fluctuations in the enzymatic reaction of HIV-1 protease"
S. Piana, P. Carloni and M. Parrinello
J. Mol. Biol. **319**, 567 (2002)
293. "Structure and chemical activity of point defects on MgCl_2 (001) surface"
K. Costuas and M. Parrinello
J. Phys. Chem. B **106**, 4477 (2002)
294. "Anharmonic Raman spectra in high-pressure ice from *ab initio* simulations"
A. Putrino and M. Parrinello
Phys. Rev. Lett. **88**, 176401 (2002)

295. "Classical polarizable force fields parametrized from *ab initio* calculations"
G. Tabacchi, C. J. Mundy, J. Hutter and M. Parrinello
J. Chem. Phys. **117**, 1416 (2002)
296. "The nature and transport mechanism of hydrated hydroxide ions in aqueous solution"
M. E. Tuckerman, D. Marx and M. Parrinello
Nature **417**, 925 (2002)
297. "Car-Parrinello study of Ziegler-Natta heterogeneous catalysis: stability and destabilization problems of the active site models"
M. Boero, M. Parrinello, K. Terakura and H. Weiss
Mol. Phys. **100**, 2935 (2002)
298. "Protonation state of the equatorial ligands and dynamics of the OH...O units in a cobaloxime biomimetic"
C. Rovira, K. Kunc and M. Parrinello
Inorg. Chem. **41**, 4810 (2002)
299. "Pulling monatomic gold wires with single molecules: an *ab initio* simulation"
D. Krüger, H. Fuchs, R. Rousseau, D. Marx and M. Parrinello
Phys. Rev. Lett. **89**, 186402 (2002)
300. "Ab-initio study of NMR chemical shifts of water under normal and supercritical conditions"
D. Sebastiani and M. Parrinello
ChemPhysChem **3**, 675 (2002)
301. "Escaping free-energy minima"
A. Laio and M. Parrinello
Proc. Natl. Acad. Sci. **99**, 12562 (2002)
302. "Electronic structure of wet DNA"
F. L. Gervasio, P. Carloni and M. Parrinello
Phys. Rev. Lett. **89**, 108102 (2002)
303. "Comment on 'Dissociation of water under pressure'"
C. Dellago, P. L. Geissler, D. Chandler, J. Hutter and M. Parrinello
Phys. Rev. Lett. **89**, 199601 (2002)
304. "*Ab initio* x-ray scattering of liquid water"
M. Krack, A. Gambirasio and M. Parrinello
J. Chem. Phys. **117**, 9409 (2002)
305. "Pressure-induced structural transformations in a medium-sized silicon nanocrystal by tight-binding molecular dynamics"
R. Martoňák, L. Colombo, C. Molteni and M. Parrinello
J. Chem. Phys. **117**, 11329 (2002)
306. "NMR chemical shifts in periodic systems from first principles"
D. Sebastiani, G. Goward, I. Schnell and M. Parrinello
Comp. Phys. Comm. **147**, 707 (2002)

307. “The role and perspective of *ab initio* molecular dynamics in the study of biological systems”
P. Carloni, U. Röthlisberger and M. Parrinello
Acc. Chem. Res. **35**, 455 (2002)
308. “A field-theoretical approach to simulation in the classical canonical and grand canonical ensemble”
S. A. Baeurle, R. Martoňák and M. Parrinello
J. Chem. Phys. **117**, 3027 (2002)
309. “Wave-function localization in reciprocal space”
M. Iannuzzi and M. Parrinello
Phys. Rev. B **66**, 155209 (2002)
310. “Solvation structure and mobility mechanism of OH⁻: A Car-Parrinello molecular dynamics investigation of alkaline solutions”
B. Chen, I. Ivanov, J. M. Park, M. Parrinello and M. L. Klein
J. Phys. Chem. B **106**, 12006 (2002)
311. “First-principles study of aqueous hydroxide solutions”
B. Chen, J. M. Park, I. Ivanov, G. Tabacchi, M. L. Klein and M. Parrinello
J. Am. Chem. Soc. **124**, 8534, (2002)
312. “First principles molecular dynamics study of catalysis for polyolefins: the Ziegler-Natta heterogeneous system”
M. Boero, K. Terakura and M. Parrinello
Int. J. Mol. Sci. **3**, 395 (2002)
313. “*Ab initio* molecular dynamics simulation of hydrogen fluoride at several thermodynamic states”
M. Kreitmeir, H. Bertagnolli, J. J. Mortensen and M. Parrinello
J. Chem. Phys. **118**, 3639 (2003)
314. “Predicting crystal structures: the Parrinello-Rahman method revisited”
R. Martoňák, A. Laio and M. Parrinello
Phys. Rev. Lett. **90**, 075503 (2003)
315. “A concerted variational strategy for investigating rare events”
D. Passerone, M. Ceccarelli and M. Parrinello
J. Chem. Phys. **118**, 2025 (2003)
316. “Water structure as a function of temperature from X-ray scattering experiments and *ab initio* molecular dynamics”
G. Hura, D. Russo, R. M. Glaeser, T. Head-Gordon, M. Krack and M. Parrinello
Phys. Chem. Chem. Phys. **5**, 1981 (2003)
317. “Efficient exploration of reactive potential energy surfaces using Car-Parrinello molecular dynamics”
M. Iannuzzi, A. Laio and M. Parrinello
Phys. Rev. Lett. **90**, 238302 (2003)

318. “*Ab initio* simulation of water interaction with the (100) surface of pyrite”
A. Stirling, M. Bernasconi and M. Parrinello
J. Chem. Phys. **118**, 8917 (2003)
319. “Comment on ‘Action-derived molecular dynamics in the study of rare events’ - Reply”
D. Passerone and M. Parrinello
Phys. Rev. Lett. **90**, 089802 (2003)
320. “First-principles molecular-dynamics simulations of a hydrated electron in normal and supercritical water”
M. Boero, M. Parrinello, K. Terakura, T. Ikeshoji and C. C. Liew
Phys. Rev. Lett. **90**, 226403 (2003)
321. “Influence of outer-shell metal ligands on the structural and electronic properties of horse liver alcohol dehydrogenase zinc active site”
F. L. Gervasio, V. Schettino, S. Mangani, M. Krack, P. Carloni and M. Parrinello
J. Phys. Chem. B. **107**, 6886 (2003)
322. “Hydrogen bonding in water”
B. Chen, I. Ivanov, M. L. Klein and M. Parrinello
Phys. Rev. Lett. **91**, 215503 (2003)
323. “*Ab initio* simulation of H₂S adsorption on the (100) surface of pyrite”
A. Stirling, M. Bernasconi and M. Parrinello
J. Chem. Phys. **119**, 4934 (2003)
324. “Insights into the electronic dynamics in chemical reactions”
D. Aktah, D. Passerone and M. Parrinello
J. Phys. Chem. A **108**, 848 (2004)
325. “Hydrogen bond driven chemical reactions: Beckmann rearrangement of cyclohexanone oxime into ϵ -caprolactam in supercritical water”
M. Boero, T. Ikeshoji, C. C. Liew, K. Terakura and M. Parrinello
J. Am. Chem. Soc. **126**, 6280 (2004)
326. “Proton transfer in heterocycle crystals”
M. Iannuzzi and M. Parrinello
Phys. Rev. Lett. **93**, 025901 (2004)
327. “Dispersion corrections to density functionals for water aromatic interactions”
U. Zimmerli, M. Parrinello and P. Koumoutsakos
J. Chem. Phys. **120**, 2693 (2004)
328. “Polyamorphism of ice at low temperatures from constant-pressure simulations”
R. Martoňák, D. Donadio and M. Parrinello
Phys. Rev. Lett. **92**, 225702 (2004)

329. "Effective force fields for condensed phase systems from *ab initio* molecular dynamics simulation: A new method for force-matching"
S. Izvekov, M. Parrinello, C. J. Burnham and G. A. Voth
J. Chem. Phys. **120**, 10896 (2004)
330. "Ab initio study of dehydroxylation-carbonation reaction on brucite surface"
S. V. Churakov, M. Iannuzzi and M. Parrinello
J. Phys. Chem. B **108**, 11567 (2004)
331. "Reconstructing the density of states by history-dependent metadynamics"
C. Micheletti, A. Laio and M. Parrinello
Phys. Rev. Lett. **92**, 170601 (2004)
332. "Microscopic mechanism of antibiotics translocation through a porin"
M. Ceccarelli, C. Danelon, A. Laio and M. Parrinello
Biophys. J. **87**, 58 (2004)
333. "A minimum free energy reaction path for the E2 reaction between fluoro ethane and a fluoride ion"
B. Ensing, A. Laio, F. L. Gervasio, M. Parrinello and M. L. Klein
J. Am. Chem. Soc. **126**, 9492 (2004)
334. "Liquid water from first principles: investigation of different sampling approaches"
I.-F. W. Kuo, C. J. Mundy, M. J. McGrath, J. I. Siepmann, J. VandeVondele, M. Sprik, J. Hutter, B. Chen, M. L. Klein, F. Mohamed, M. Krack and M. Parrinello
J. Phys. Chem. B **108**, 12990 (2004)
335. "Correlations among hydrogen bonds in liquid water"
P. Raiteri, A. Laio and M. Parrinello
Phys. Rev. Lett. **93**, 087801 (2004)
336. "Molecular dynamics simulation of reconstructive phase transitions on an anhydrous zeolite"
C. Ceriani, A. Laio, E. Fois, A. Gamba, R. Martoňák and M. Parrinello
Phys. Rev. B **70**, 113403 (2004)
337. "Influence of DNA structure on the reactivity of the guanine radical cation"
F. L. Gervasio, A. Laio, M. Iannuzzi and M. Parrinello
Chem. Eur. J. **10**, 4846 (2004)
338. "Azulene-to-naphthalene rearrangement: The Car-Parrinello metadynamics method explores various mechanisms"
A. Stirling, M. Iannuzzi, A. Laio and M. Parrinello
Chem. Phys. Chem. **5** (10), 1558 (2004)
339. "Solvation states of HCl in mixed ether: acid crystals: A computational study"
V. Buch, F. Mohamed, M. Krack, J. Sadlej, J.P. Devlin and M. Parrinello
J. Chem. Phys. **121** (24), 12135-12138 (2004)

340. "The influence of temperature and density functional models in ab initio molecular dynamics simulation of liquid water"
J. VandeVondele, F. Mohamed, M. Krack, J. Hutter, M. Sprik and M. Parrinello
J. Chem. Phys. **122** (1), 2005 Art. No 014515
341. "Flexible docking in solution using metadynamics"
F. L. Gervasio, A. Laio and M. Parrinello
J. Am. Chem. Soc. **127** (8), 2600-2607 (2005)
342. "A recipe for the computation of the free energy barrier and the lowest free energy path of concerted reactions"
B. Ensing, A. Laio, M. Parrinello and M. Klein
J. Phys. Chem. B **109** (14), 6676-6687 (2005)
343. "Topological defects and bulk melting of hexagonal ice"
D. Donadio, P. Raiteri and M. Parrinello
J. Phys. Chem. B **109**, (12), 5421-5424 (2005)
344. "Assessing the accuracy of metadynamics"
A. Laio, A. Rodriguez-Forteza, F. L. Gervasio, M. Ceccarelli and M. Parrinello
J. Phys. Chem. B **109**, (14), 6714-6721 (2005)
345. "Simulation of structural phase transitions by metadynamics"
R. Martoňák, A. Laio, M. Bernasconi, C. Cerini, P. Raiteri, F. Zipoli and M. Parrinello
Zeitschrift für Kristallographie **220**, 489-498 (2005)
346. "Evolution of the structure of amorphous ice: From low-density amorphous through high-density amorphous to very high-density amorphous ice"
R. Martoňák, D. Donadio and M. Parrinello
J. Chem. Phys. **122** (13), Art. No 134501 (2005)
347. "Charge Localization in DNA Fibers"
F. L. Gervasio, A. Laio and M. Parrinello
Phys. Rev. Lett. **94** (15), Art.No 158103 (2005)
348. "Toward a Monte Carlo program for simulating vapor-liquid phase equilibria from first principles"
M. J. McGrath, J. Ilja Siepmann, I-Feng W. Kuo, C. J. Mundy, J. VandeVondele, M. Sprik, J. Hutter, F. Mohamed, M. Krack and M. Parrinello
Comp. Phys. Comm. **169**, 289-294 (2005)
349. "Experimental and computational study of isotopic effects within the Zundel ion"
J.P. Devlin, M.W. Severson, F. Mohamed, J. Sadlej, V. Buch and M. Parrinello
Chem. Phys. Lett. **408**, 439-444 (2005)
350. "QUICKSTEP: Fast and accurate density functional calculations using a mixed Gaussian and plane waves approach"
J. VandeVondele, M. Krack, F. Mohamed, M. Parrinello, T. Chassaing and J. Hutter
Comp. Phys. Comm. **167**, (2), 103-128 (2005)

351. "Exploring polymorphism: The case of benzene"
P. Raiteri, R. Martoňák and M. Parrinello
Angew. Chemie, Internat.Edition **44** (24), 3769-3773 (2005)
352. "The role of the peripheral anionic site and cation-pi interactions in the ligand penetration of the human AChE gorge"
D. Branduardi, F. L. Gervasio, A. Cavalli, M. Recanatini and M. Parrinello
J. Am. Chem. Soc. **127** (25), 9147-9155 (2005)
353. "Beta-Lactone synthesis from epoxide and CO: Reaction mechanism revisited"
A. Stirling, M. Iannuzzi, M. Parrinello, F. Molnar, V. Bernhart and G. A. Luinstra
Organometallics **24** (10), 2533-2537 (2005)
354. "Stochastic linear scaling for metals and nonmetals"
F. R. Krajewski and M. Parrinello
Phys. Rev. B **71** (23), Art. No. 233105 (2005)
355. "Nonperiodic boundary conditions for solvated systems"
G. Petraglio, M. Ceccarelli and M. Parrinello
J. Chem. Phys. **123** (4), Art. No 044103 (2005)
356. "A new molecular-dynamics based approach for molecular crystal structure search"
V. Buch, R. Martoňák and M. Parrinello
J. Chem. Phys. **123** (5), Art. No 051108 (2005)
357. "The microscopic switching mechanism of a [2]catenane"
M. Ceccarelli, F. Mercuri, D. Passerone and M. Parrinello
J. Phys. Chem. B **109** (36), 17094-17099 (2005)
358. "Anisotropy of Earth's D" layer and stacking faults in the MgSiO₃ post-perovskite phase"
A. R. Oganov, R. Martoňák, A. Laio, P. Raiteri and M. Parrinello
Nature **438**, 1142-1144 (2005)
359. "An efficient real space multigrid QM/MM electrostatic coupling"
T. Laino, F. Mohamed, A. Laio and M. Parrinello
J. Chem. Theory Comput. **1** (6), 1176-1184 (2005)
360. "Lithium hydroxide phase transition under high pressure: An ab initio molecular dynamics study"
M. Pagliai, M. Iannuzzi, G. Cardini, M. Parrinello and V. Schettino
Chem. Phys. Chem. **7** (1), 141-145 (2006)
361. "Linear scaling electronic structure calculations and accurate statistical mechanics sampling with noisy forces"
F. R. Krajewski and M. Parrinello
Phys. Rev. B **73**, 041105, (2006)

362. “Metadynamics simulation of prion protein: β -structure stability and the early stages of misfolding”
A. Barducci, R. Chelli, P. Procacci, V. Schettino, F. L. Gervasio and M. Parrinello
J. Am. Chem. Soc. **128** (8), 2705-2720 (2006)
363. “Ab initio molecular dynamics study of heterogeneous oxidation of graphite by means of gas-phase nitric acid”
A. Rodriguez-Forteza, M. Iannuzzi and M. Parrinello
J. Phys. Chem. B **110** (8), 3477 (2006)
364. “Efficient reconstruction of complex free energy landscapes by multiple walkers metadynamics”
P. Raiteri, A. Laio, F. L. Gervasio, C. Micheletti and M. Parrinello
J. Phys. Chem. B **110** (8), 3533 (2006)
365. “Equilibrium free energies from nonequilibrium metadynamics”
G. Bussi, A. Laio and M. Parrinello
Phys. Rev. Lett. **96** (9), 090601 (2006)
366. “A QUICKSTEP-based quantum mechanics/molecular mechanics approach for silica”
F. Zipoli, T. Laino, A. Laio, M. Bernasconi and M. Parrinello
J. Chem. Phys. **124** (15), 154707 (2006)
367. “Exploration of NVE classical trajectories as a tool for molecular crystal structure prediction, with tests on ice polymorphs”
V. Buch, R. Martoňák and M. Parrinello
J. Chem. Phys. **124** (20), 204705 (2006)
368. “Non-equilibrium dynamics and structure of interfacial ice”
O. Andreussi, D. Donadio, M. Parrinello and A. H. Zewail
Chem. Phys. Lett. **426** (1-3), 115-119, (2006)
369. “Crystal structure transformations in SiO_2 from classical and *ab initio* metadynamics”
R. Martoňák, D. Donadio, A. R. Oganov and M. Parrinello
Nature Materials **5**, (8), 623-626 (2006)
370. “Exploring the gating mechanism in the CIC chloride channel *via* metadynamics”
F. L. Gervasio, M. Parrinello, M. Ceccarelli and M. L. Klein
J. Mol. Biol. **361** (2), 390-398 (2006)
371. “Dissociation mechanism of acetic acid in water”
J. M. Park, A. Laio, M. Iannuzzi and M. Parrinello
J. Am. Chem. Soc. **128** (35), 11318-11319 (2006)
372. “Double proton coupled charge transfer in DNA”
F. L. Gervasio, M. Boero and M. Parrinello
Angew. Chem. Int. Ed. **45** (34): 5606-5609 (2006)

373. “An efficient linear-scaling electrostatic coupling for treating periodic boundary conditions in QM/MM simulations”
T. Laino, F. Mohamed, A. Laio and M. Parrinello
J. Chem. Theory Comput. **2** (5), 1370-1378 (2006)
374. “Freezing of a Lennard-Jones fluid: From nucleation to spinodal regime”
F. Trudu, D. Donadio and M. Parrinello
Phys. Rev. Lett. **97** (10), 105701 (2006)
375. “Using metadynamics to understand the mechanism of calmodulin/target recognition at atomic detail”
G. Fiorin, A. Pastore, P. Carloni and M. Parrinello
J. Biophys. **91** (8), 2768-2777 (2006)
376. “Linear scaling for quasi-one-dimensional systems”
F. R. Krajewski and M. Parrinello
Phys. Rev. B **74** (12), 125107 (2006)
377. “Stability and structure of oligomers of the Alzheimer peptide $A\beta_{16-22}$: From the dimer to the 32-Mer”
U. F. Röhrig, A. Laio, N. Tantalo, M. Parrinello and R. Petronzio
Biophysical Journal **91** (9), 3217-3229 (2006)
378. “Free-energy landscape for β hairpin folding from combined parallel tempering and metadynamics”
G. Bussi, F. L. Gervasio, A. Laio and M. Parrinello
J. Am. Chem. Soc. **128** (41), 13435-13441 (2006)
379. “The amorphous analogs of the crystalline monohydrate of HCl: Structures and spectra”
J. P. Devlin, V. Buch, F. Mohamed and M. Parrinello
Chem. Phys. Lett. **432**, 462-467 (2006)
380. “Canonical sampling through velocity rescaling”
G. Bussi, D. Donadio and M. Parrinello
J. Chem. Phys. **126**, 014101 (2007)
381. “Charge Localization in Stacked Radical Cation DNA Base Pairs and the Benzene Dimer Studied by Self-Interaction Corrected Density-Functional Theory”
Y. A. Mantz, F. L. Gervasio, T. Laino and M. Parrinello
J. Phys. Chem. A **111**, 105-112 (2007)
382. “A new glance at HCl-monohydrate spectroscopy, using on-the-fly dynamics”
V. Buch, F. Mohamed, J. P. Devlin and M. Parrinello
J. Chem. Phys. **126**, 021102 (2007)
383. “From *A* to *B* in free energy space”
D. Branduardi, F. L. Gervasio and M. Parrinello
J. Chem. Phys. **126**, 054103 (2007)

384. “Efficient and accurate Car-Parrinello-like approach to Born-Oppenheimer Molecular Dynamics”
T. D. Kühne, M. Krack, F. Mohamed and M. Parrinello
Phys. Rev. Lett. **98**, 066401 (2007)
385. “Elusive structure of HCl monohydrate”
V. Buch, F. Mohamed, M. Parrinello and J. P. Devlin
J. Chem. Phys. **126**, 074503 (2007)
386. “Free energy ab initio metadynamics: A new tool for the theoretical study of organometallic reactivity? Example of the C-C and C-H reductive eliminations from platinum(IV) complexes”
C. Michel, A. Laio, F. Mohamed, M. Krack, M. Parrinello and A. Milet
Organometallics **26**, 1241-1249 (2007)
387. “Charge localisation and hopping in DNA”
M. Boero, F. L. Gervasio and M. Parrinello
Molecular Simulation **33** (1-2), 57-60 (2007)
388. “Ab initio molecular dynamics study of heterogeneous Nitric acid decomposition reactions on graphite surfaces”
A. Rodriguez-Fortea, M. Iannuzzi and M. Parrinello
J. Phys. Chem. C **111**, 2251-2258 (2007)
389. “Generalized neural-network representation of high-dimensional potential-energy surfaces”
J. Behler and M. Parrinello
Phys. Rev. Lett. **98** (14), 146401 (2007)
390. “Defective pyrite (100) surface: An ab initio study”
A. Stirling, M. Bernasconi and M. Parrinello
Phys. Rev. B **75** (16), 165406 (2007)
391. “The interplay between surface-water and hydrogen bonding in a water adlayer on Pt(111) and Ag(111)”
L. Delle Site, L. M. Ghiringhelli, O. Andreussi, D. Donadio and M. Parrinello
J. Phys. Condens. Matter **19**, 242101 (2007)
392. “Accurate sampling using Langevin dynamics”
G. Bussi and M. Parrinello
Phys. Rev. E **75**, 056707 (2007)
393. ““Site binding” of Ca²⁺ Ions to Polyacrylates in water: A molecular dynamics study of coiling an aggregation”
R. E. Bulo, D. Donadio, A. Laio, F. Molnar, J. Rieger and M. Parrinello
Macromolecules **40**, 3437-3442 (2007)
394. “Energy conservation in adaptive hybrid atomistic/coarse-grain molecular dynamics”
B. Ensing, S. O. Nielsen, P. B. Moore, M. L. Klein and M. Parrinello
J. Chem. Theory Comput. **3**, 1100-1105 (2007)

395. "From four- to six-coordinated silica: Transformation pathways from metadynamics"
R. Martoňák, D. Donadio, A. R. Oganov and M. Parrinello
Phys. Rev. B **76**, 014120 (2007)
396. "The conformational free energy landscape of β -D-Glucopyranose. Implications for substrate preactivation in β -Glucoside hydrolases"
X. Biarnes, A. Ardèvol, A. Planas, C. Rovira, A. Laio and M. Parrinello
J. Am. Chem. Soc. **129** (35), 10686-10693 (2007)
397. "Linear scaling electronic structure Monte Carlo method for metals"
F. R. Krajewski and M. Parrinello
Phys. Rev. B **75**, 235108 (2007)
398. "Solvent effects on charge spatial extent in DNA and implications for transfer"
Y. A. Mantz, F. L. Gervasio, T. Laino and M. Parrinello
Phys. Rev. Lett. **99**, 058104 (2007)
399. "Conjugate gradient heat bath for ill-conditioned actions"
M. Ceriotti, G. Bussi and M. Parrinello
Phys. Rev. E **76**, 026707 (2007)
400. "Insight into the folding inhibition of HIV-1 protease by a small peptide"
M. Bonomi, F. L. Gervasio, G. Tiana, D. Provasi, R. A. Broglia and M. Parrinello
Biophysical Journal **93** (8), 2813-2821 (2007)
401. "Molecular dynamics study of the solvation of calcium carbonate in water"
F. Bruneval, D. Donadio and M. Parrinello
J. Phys. Chem. B. **111** (42), 12219-12227 (2007)
402. "Coexistence of tetrahedral- and octahedral-like sites in amorphous phase change materials"
S. Caravati, M. Bernasconi, T. D. Kühne, M. Krack and M. Parrinello
Applied Phys. Lett. **91** 171906 (2007)
403. "At the water's edge: Nitric acid as a weak acid"
E. S. Shamay, V. Buch, M. Parrinello and G. L. Richmond
J. Am. Chem. Soc. **129**, 12910-12911 (2007)
404. "The role of Li^+ , Na^+ , and K^+ in the ligand binding inside the human acetylcholinesterase gorge"
G. Petraglio, M. Bartolini, D. Branduardi, V. Andrisano, M. Recanatini, F. L. Gervasio, A. Cavalli and M. Parrinello
Proteins **70**, 779-785 (2008)
405. "Well-tempered metadynamics: a smoothly converging and tunable free-energy method"
A. Barducci, G. Bussi and M. Parrinello
Phys. Rev. Lett. **100**, 0206003 (2008)

406. "Influence of temperature and anisotropic pressure on the phase transitions in α -Cristobalite"
D. Donadio, R. Martoňák, P. Raiteri and M. Parrinello
Phys. Rev. Lett. **100** (16), 165502 (2008)
407. "The thermal stability of lattice-energy minima of 5-Fluorouracil: metadynamics as an aid to polymorph prediction"
P. G. Karamertzanis, P. Raiteri, M. Parrinello, M. Leslie and S. L. Price
J. Phys. Chem. B **112**, 4298-4308 (2008)
408. "HCl Hydrates as model systems for protonated water"
V. Buch, A. Dubrovskiy, F. Mohamed, M. Parrinello, J. Sadlej, A. D. Hammerich and J. P. Devlin
J. Phys. Chem. A **112**, 2144-2161 (2008)
409. "Unravelling the shuttling mechanism in a photoswitchable multicomponent bistable rotaxane"
P. Raiteri, G. Bussi, C. S. Cucinotta, A. Credi, J. F. Stoddart and M. Parrinello
Angew. Chemie, Int. Ed. **47** (19), 3536-3539 (2008)
410. "Metadynamics simulations of the high-pressure phases of Silicon employing a high-dimensional neural network potential"
J. Behler, R. Martoňák, D. Donadio and M. Parrinello
Phys. Rev. Lett. **100**, 185501 (2008)
411. "DFT research on the Dehydroxylation reaction of Pyrophyllite 1. first-principle molecular dynamics simulation"
E. Molina-Montes, D. Donadio, A. Hernandez-Laguna, C. I. Saint-Diaz and M. Parrinello
J. Phys. Chem. B **112**, 7051-7060 (2008)
412. "Anharmonic infrared and Raman spectra in Car-Parrinello molecular dynamics simulations"
M. Pagliai, C. Cavazzoni, G. Cardini, G. Erbacci, M. Parrinello and V. Schettino
J. Chem. Phys. **128**, 224514 (2008)
413. "Stochastic thermostats: comparison of local and global schemes"
G. Bussi and M. Parrinello
Comp. Phys. Comm. **179**, 26-29 (2008)
414. "Conformational changes and gating at the selectivity filter of Potassium channels"
C. Domene, M. L. Klein, D. Branduardi, F. L. Gervasio and M. Parrinello
J. Am. Chem. Soc. **130**, 9474-9480 (2008)
415. "New Lennard-Jones metastable phase"
H. Eshet, F. Bruneval and M. Parrinello
J. Chem. Phys. **129**, 026101 (2008)
416. "An efficient and accurate decomposition of the Fermi operator"
M. Ceriotti, T. D. Kühne and M. Parrinello
J. Chem. Phys. **129**, 024707 (2008)

417. “The unfolded ensemble and folding mechanism of the C-terminal BG1 β -hairpin”
M. Bonomi, D. Branduardi, F. L. Gervasio and M. Parrinello
J. Am. Chem. Soc. **130** (42), 13938-13944 (2008)
418. “Vacancy-vacancy interaction and oxygen diffusion in stabilized cubic ZrO₂ from first principles”
F. Pietrucci, M. Bernasconi, A. Laio and M. Parrinello
Phys. Rev. B **78** (9), 094301 (2008)
419. “Investigating the polymorphism in PR179: a combined crystal structure prediction and metadynamics study”
T. Zykova-Timan, P. Raiteri and M. Parrinello
J. Phys. Chem B. **112** (42), 13231-13237 (2008)
420. “Modeling the hydrogen storage materials with exposed M²⁺ coordination sites”
M. Kosa, M. Krack, A. K. Cheetham and M. Parrinello
J. Phys. Chem. C **112** (42), 16171-16173 (2008)
421. “Pressure-induced phase transitions in silicon studied by neural network-based metadynamics simulations”
J. Behler, R. Martoňák, D. Donadio and M. Parrinello
Phys. Stat. Sol. (b) **245** (12), 2618-2629 (2008)
422. “Langevin equation with colored noise for constant-temperature molecular dynamics simulations”
M. Ceriotti, G. Bussi and M. Parrinello
Phys. Rev. Lett. **102** (2), 020601 (2009)
423. “Static and dynamical properties of liquid water from first principles by a novel Car-Parrinello-like approach”
T. D. Kuehne, M. Krack and M. Parrinello
J. Chem. Theory Comput. **5** (2), 235-241 (2009)
424. “Isothermal-isobaric molecular dynamics using stochastic velocity rescaling”
G. Bussi, T. Zykova-Timan and M. Parrinello
J. Chem. Phys. **130** (7), 074101 (2009)
425. “Protein conformational transitions: the closure mechanism of a kinase explored by atomistic simulations”
A. Berteotti, A. Cavalli, D. Branduardi, F. L. Gervasio, M. Recanatini and M. Parrinello
J. Am. Chem. Soc. **131** (1), 244-250 (2009)
426. “Binding of Calcium and Carbonate to Polyacrylates”
G. A. Tribello, C. C. Liew and M. Parrinello
J. Phys. Chem. B **113** (20), 7081-7085 (2009)
427. “Unravelling the mechanism of pressure induced amorphization of phase change materials”
S. Caravati, M. Bernasconi, T. D. Kühne, M. Krack and M. Parrinello
Phys. Rev. Lett. **102** (20), 205502 (2009)

428. “First-principles study of crystalline and amorphous Ge₂Sb₂Te₂ and the effects of stoichiometric defects”
S. Caravati, M. Bernasconi, T. D. Kühne, M. Krack and M. Parrinello
J. Phys. Condens. Matter **21** (25), 255501 (2009)
429. “Reconstructing the equilibrium Boltzmann distribution from well-tempered metadynamics”
M. Bonomi, A. Barducci and M. Parrinello
J. Comput. Chem. **30** (11), 1615-1621 (2009)
430. “Nucleotide-dependent conformational states of actin”
J. Pfandtner, D. Branduardi, M. Parrinello, T. D. Pollard and G. A. Voth
PNAS **106** (31), 12723-12728 (2009)
431. “Nuclear quantum effects in solids using a colored-noise thermostat”
M. Ceriotti, G. Bussi and M. Parrinello
Phys. Rev. Lett. **103** (3), 030603 (2009)
432. “A molecular dynamics study of the early stages of calcium carbonate growth”
G. A. Tribello, F. Bruneval, C. C. Liew and M. Parrinello
J. Phys. Chem. B **113** (34), 11680-11687 (2009)
433. “Superionic conduction in substoichiometric LiAl alloy: an *ab initio* study”
C. S. Cucinotta, G. Miceli, P. Raiteri, M. Krack, T. D. Kühne, M. Bernasconi and M. Parrinello
Phys. Rev. Lett. **103**, (12), 125901 (2009)
434. “Ensemble of transition state structures for the Cis-Trans Isomerization of N-Methylacetamide”
Y. A. Mantz, D. Branduardi, G. Bussi and M. Parrinello
J. Phys. Chem. B **112** (37), 12521-12529 (2009)
435. “PLUMED: A portable plugin for free-energy calculations with molecular dynamics”
M. Bonomi, D. Branduardi, G. Bussi, C. Camilloni, D. Provasi, P. Raiteri, D. Donadio, F. Marinelli, F. Pietrucci, R. A. Broglia and M. Parrinello
Comp. Phys. Comm. **180** (10), 1961-1972 (2009)
436. “Phase selection and energetics in chiral alkaline earth tartrates and their racemic and *meso* analogues: Synthetic, structural, computational, and calorimetric studies”
L. N. Appelhans, M. Kosa, A. V. Radha, P. Simoncic, A. Navrotsky, M. Parrinello and A. K. Cheetham
J. Am. Chem. Soc. **131** (42), 15375-15386 (2009)
437. “First-principles study of liquid and amorphous Sb₂Te₃”
S. Caravati, M. Bernasconi and M. Parrinello
Phys. Rev. B **81**, 014201 (2010)
438. “A hybrid approach to Fermi operator expansion”
M. Ceriotti, T. D. Kühne and M. Parrinello
AIP Conference Proceedings, 658-61 (2009)

439. “Signature of tetrahedral Ge in the Raman spectrum of amorphous phase-change materials“
R. Mazzarello, S. Caravati, S. Angioletti-Uberti, M. Bernasconi and M. Parrinello
Phys. Rev. Lett. **104**, 085503 (2010)
440. “Molecular basis of cyclooxygenase enzymes (COXs) selective inhibition“
V. Limongelli, M. Bonomi, L. Marinelli, F. L. Gervasio, A. Cavalli, E. Novellino and M. Parrinello
PNAS **107** (12), 5411-5416 (2010)
441. “Graphite-diamond phase coexistence study employing a neural-network mapping of the ab initio potential energy surface“
R. Z. Khaliullin, H. Eshet, T. D. Kühne, J. Behler and M. Parrinello
Phys. Rev. B **81** (10), 100103 (2010)
442. “Colored-noise thermostats à la carte“
M. Ceriotti, G. Bussi and M. Parrinello
J. Chem. Theory and Computation (JCTC) **6** (4), 1170-1180 (2010)
443. “*Ab initio* quality neural-network potential for sodium“
H. Eshet, R. Z. Khaliullin, T. D. Kühne, J. Behler and M. Parrinello
Phys. Rev. B **81** (18), 184107 (2010)
444. “Enhanced sampling in the well-tempered ensemble“
M. Bonomi and M. Parrinello
Phys. Rev. Lett. **104** (19), 190601 (2010)
445. “Linking well-tempered metadynamics simulations with experiments“
A. Barducci, M. Bonomi and M. Parrinello
Biophysical Journal **10**, L44-L46 (2010)
446. “Targeting biomolecular flexibility with metadynamics“
V. Leone, F. Marinelli, P. Carloni and M. Parrinello
Structural Biology **20**, 148-154 (2010)
447. “Probing the mechanism of pH-induced large-scale conformational changes in dengue virus envelope protein using atomistic simulations“
M. K. Prakash, A. Barducci and M. Parrinello
Biophysical Journal **99**, (2), 588-594 (2010)
448. “First principles study of the optical contrast in phase change materials“
S. Caravati, M. Bernasconi and M. Parrinello
J. Phys. Condensed Matter **22** (31), 315801 (2010)
449. “Asprich peptides are occluded in calcite and permanently disorder biomineral crystals“
R. A. Metzler, G. A. Tribello, M. Parrinello and P. U. P. A. Gilbert
J. Am. Chem. Soc. **132** (33) 11585-11591 (2010)

450. “Displaced path integral formulation for the momentum distribution of quantum particles”
L. Lin, J. A. Morrone, R. Car and M. Parrinello
Phys. Rev. Lett. **105** (11), 110602 (2010)
451. “Probing the mechanical properties of hybrid inorganic-organic frameworks: a computational and experimental study”
M. Kosa, J. C. Tan, C. A. Merrill, M. Krack, A. K. Cheetham and M. Parrinello
ChemPhysChem **11** (11), 2332-2336 (2010)
452. “A method to break all barriers”
F. Pulizzi and M. Parrinello
Nature Materials **9** (9), 693-694 (2010) Interview
453. “A model approach to modeling”
R. Car and M. Parrinello
Nature Materials **9** (9), 687 (2010)
454. “Multiple routes and milestones in the folding of HIV-1 protease monomer”
M. Bonomi, A. Barducci, F. L. Gervasio and M. Parrinello
PLoS ONE **5** (10), 13208 (2010)
455. “Efficient stochastic thermostating of path integral molecular dynamics”
M. Ceriotti, M. Parrinello, T. E. Markland and D. E. Manolopoulos
J. Chem. Phys. **133**, 124104 (2010)
456. “The delta-thermostat: selective normal-modes excitation by colored-noise Langevin dynamics”
M. Ceriotti and M. Parrinello
Proceedings: International Conference on Computational Science, ICCS 2010
Procedia Computer Science **1**, 1607-1614 (2010)
457. “A self-learning algorithm for biased molecular dynamics”
G. A. Tribello, M. Ceriotti and M. Parrinello
PNAS **107** (41), 17509-17514 (2010)
458. “First principles study of the $\text{LiNH}_2/\text{Li}_2\text{NH}$ transformation”
G. Miceli, C. S. Cucinotta, M. Bernasconi and M. Parrinello
J. Phys. Chem. C **114** (35), 15174-15183 (2010)
459. “Nuclear quantum effects in *ab initio* dynamics: theory and experiments for lithium imide”
M. Ceriotti, G. Miceli, A. Pietropaolo, D. Colognesi, A. Nale, M. Catti, M. Bernasconi and M. Parrinello
Phys. Rev. B **82**, 174306 (2010)
460. “Static disorder and structural correlations in the low-temperature phase of lithium imide”
G. Miceli, M. Ceriotti, M. Bernasconi and M. Parrinello
Phys. Rev. B **83**, 054119 (2011)

461. “Structural diversity and energetic in anhydrous lithium tartrates: experimental and computational studies of novel chiral polymorphs and their racemic and meso analogues”
H. H.-M. Yeung, M. Kosa, M. Parrinello, P. M. Forster and A. K. Cheetham
Crystal Growth & Design **11**, 221 – 230 (2011)
462. “Accelerating the convergence of path integral dynamics with a generalized Langevin equation”
M. Ceriotti, D. E. Manolopoulos and M. Parrinello
J. Chem. Phys **134**, 084104 (2011)
463. “First-principles study of the high-temperature phase of Li_2NH ”
G. Miceli, M. Ceriotti, S. Angioletti-Uberti, M. Bernasconi and M. Parrinello
J. Phys. Chem. C **115**, 7076-7080 (2011)
464. “Momentum distribution, vibrational dynamics, and the potential of mean force in ice”
L. Lin, J. A. Morrone, R. Car and M. Parrinello
Phys. Rev. B **83**, 220302 (2011)
465. “First-principles study of nitrogen doping in cubic and amorphous $\text{Ge}_2\text{Sb}_2\text{Te}_5$ ”
S. Caravati, D. Colleoni, R. Mazzarello, T. D. Kühne, M. Krack, M. Bernasconi and M. Parrinello
J. Phys. Condens. Matter **23**, 265801 (2011)
466. “Replica temperatures for uniform exchange and efficient roundtrip times in explicit solvent parallel tempering simulations”
M. K. Prakash, A. Barducci and M. Parrinello
J. of Chemical Theory and Computation **7** (7), 2025-2027 (2011)
467. “A quantitative measure of chirality inside nucleic acid databank”
A. Pietropaolo and M. Parrinello
Chirality **23** (7), 534-542 (2011)
468. “Simplifying the representation of complex free-energy landscapes using sketch-map”
M. Ceriotti, G. A. Tribello and M. Parrinello
PNAS **108** (32), 13023-13028 (2011)
469. “Nucleation mechanism for the direct graphite-to-diamond phase transition”
R. Z. Khaliullin, H. Eshet, T. D. Kuehne, J. Behler and M. Parrinello
Nature Materials **10** (9), 693-697 (2011)
470. “A Chirality-Based Metrics for Free-Energy Calculations in Biomolecular Systems”
A. Pietropaolo, D. Branduardi, M. Bonomi and M. Parrinello
J. of Comput. Chem. **32** (12), 2627-2637 (2011)
471. “Metadynamics”
A. Barducci, M. Bonomi and M. Parrinello
Comp. Mol. Sci., **1**, 826-843 (2011)
472. “Exploring the free energy surfaces of clusters using reconnaissance metadynamics”
G. A. Tribello, J. Cuny, H. Eshet and M. Parrinello
J. Chem. Phys., **135** (11), 114109 (2011)

473. "Hydrogen Oxidation Reaction at the Ni/YSZ Anode of Solid Oxide Fuel Cells from First Principles"
C. S. Cucinotta, M. Bernasconi and M. Parrinello
Phys. Rev. Lett., **107** (20), 206103 (2011)
474. "On the recombination of hydronium and hydroxide ions in water"
A. Hassanali, M. K. Prakash, H. Eshet and Michele Parrinello
PNAS, **108** (51), 20410-20415 (2011)
475. "Effect of Urea on the β -Hairpin Conformational Ensemble and Protein Denaturation Mechanism"
A. Berteotti, A. Barducci and Michele Parrinello
J. Am. Chem. Soc., **133**, 17200-17206 (2011)
476. "Counterion Redistribution upon Binding of a Tat-Protein Mimic to HIV-1 TAR RNA"
T. N. Do., E. Ippoliti, P. Carloni, G. Varani and M. Parrinello
J. of Chemical Theory and Computation, **8** (2), 688-694 (2012)
477. "Sampling protein motion and solvent effect during ligand binding"
V. Limongelli, L. Marinelli, S. Cosconati, C. La Motta, S. Sartini, L. Mugnaini, F. Da Settimo, E. Novellino and M. Parrinello
PNAS, **109** (5), 1467-1472 (2012)
478. "Investigating the Mechanism of Substrate Uptake and Release in the Glutamate Transporter Homologue Glt(Ph) through Metadynamics Simulations"
G. Grazioso, V. Limongelli, D. Branduardi, E. Novellino, C. De Micheli, A. Cavalli and M. Parrinello
J. Am. Chem. Soc., **134** (1), 453-463 (2012)
479. "Microscopic Origins of the Anomalous melting Behavior of Sodium under High Pressure"
H. Eshet, R. Z. Khaliullin, T. D. Kühne, J. Behler and M. Parrinello
Phys. Rev. Lett. **108**, 115701 (2012)
480. "Using sketch-map coordinates to analyze and bias molecular dynamics simulations"
G. A. Tribello, M. Ceriotti and M. Parrinello
PNAS, **109** (14), 5196-5201 (2012)
481. "Locating binding poses in protein-ligand systems using reconnaissance metadynamics"
P. Söderhjelm, G. A. Tribello and M. Parrinello
PNAS, **109** (14), 5170-5175 (2012)
482. "The Fuzzy Quantum Proton in the Hydrogen Chloride Hydrates"
A. A. Hassanali, J. Cuny, M. Ceriotti, C. J. Pickard and M. Parrinello
J. Am. Chem. Soc., **134**, 8557-8569 (2012)
483. "Ab Initio Molecular Dynamics Study of the Dehydroxylation Reaction in a Smectite Model"
D. Munoz-Santiburcio, M. Kosa, A. Hernandez-Laguna, C. I. Sainz-Diaz and M. Parrinello
Phys. Chem. C, **116**, 12203-12211 (2012)

484. “Metadynamics with Adaptive Gaussians”
D. Branduardi, G. Bussi and Michele Parrinello
J. Chem. Theory Comput. **8**, 2247-2254 (2012)
485. “Density functional simulations of Sb-rich GeSbTe phase change alloys”
S. Gabardi, S. Caravati, M. Bernasconi and M. Parrinello
J. Physics-Cond. Matter, **24** (38), 385803 (2012)
486. “Uncovering Molecular Details of Urea Crystal Growth in the Presence of Additives”
M. Salvalaglio, T. Vetter, F. Giberti, M. Mazzotti and M. Parrinello
J. Am. Chem. Soc., **134**, 17221-17233 (2012)
487. “Combined Computational and Experimental NMR Study of Calix[4]arene Derivatives”
V. Verdolino, L. Baldini, F. Palazzesi, F. Giberti and M. Parrinello
J. Phys. Chem. C, **116**, 23441-23452 (2012)
488. “Negative Linear Compressibility of a Metal Organic Framework”
Wei Li, Michael R. Probert, Monica Kosa, Thomas D. Bennett, A. Thirumurugan, Ryan P. Burwood, Michele Parrinello, Judith A. K. Howard and Anthony K. Cheetham
J. Am. Chem. Soc., **134**, 11940-11943 (2012)
489. “Combining metadynamics simulation and experiments to characterize dendrimers in solution”
G. M. Pavan, A. Barducci, L. Albertazzi and M. Parrinello
Soft Matter, **9**, 2593-2597(2013), DOI: 10.1039/C3SM27706B
490. “The G-Triplex DNA”
V. Limongelli, S. De Tito, L. Cerofolini, M. Fragai, B. Pagano, R. Trotta, S. Cosconati, L. Marinelli, E. Novellino, I. Bertini, A. Randazzo, C. Luchinat and M. Parrinello
Angew. Chem. Int. Ed., **52**, 2269-2273 (2013); DOI: 10.1002/anie.201206522
491. “Density functional simulations of hexagonal Ge₂Sb₂Te₅ at high pressure”
S. Caravati, G. C. Sosso, M. Bernasconi and M. Parrinello
Physical Rev. B, **87**, 094117 (2013), DOI: 10.1103/PhysRevB.87.094117
492. “Water Release from Pyrophyllite during the Dehydroxylation Process Explored by Quantum mechanical Simulations”
E. Molina-Montes, D. Donadio, A. Hernández-Laguna, M. Parrinello and C. I. Sainz-Díaz
J. Phys. Chem. C, **117**, 7526-7532 (2013); DOI: 10.1021/jp310739y
493. “Demonstrating the Transferability and the Descriptive Power of Sketch-Map”
M. Ceriotti, G. A. Tribello and M. Parrinello
J. Chem. Theory Comput., **9**, 1521-1532 (2013), DOI: 10.1021/ct3010563
494. “Funnel metadynamics as accurate binding free-energy method”
V. Limongelli, M. Bonomi and M. Parrinello
PNAS, **110** (16), 6358-6363 (2013), DOI: 10.1073/pnas.1303186110
495. “Transient Polymorphism in NaCl”
F. Giberti, G. A. Tribello and M. Parrinello
J. Chem. Theory Comp., **9** (6), 2526-2530 (2013), DOI: 10.1021/ct4002027

496. “Chiral, Racemic, and *Meso*-Lithium Tartrate Framework Polymorphs: A Detailed Structural Analysis”
H. H.-M. Yeung, M. Kosa, M. Parrinello and A. K. Cheetham
Crys. Growth Des., **13**, 3705-3715 (2013), DOI: 10.1021/cg400741b
497. “Proton transfer through the water gossamer”
A. Hassanali, F. Giberti, J. Cuny, T. D. Kühne and M. Parrinello
PNAS, **110** (34), 13723-13728 (2013), DOI: 10.1073/pnas.1306642110
498. “The allosteric communication pathways in KIX domain of CBP”
F. Palazzesi, A. Barducci, M. Tollinger and M. Parrinello
PNAS, **110** (35), 14237-14242 (2013), DOI 10.1073/pnas.1313548110
499. “Nuclear quantum effects and hydrogen bond fluctuations in water”
M. Ceriotti, J. Cuny, M. Parrinello and D. E. Manolopoulos
PNAS, **110** (39), 15591 – 15596 (2013), DOI: 10.1073/pnas.1308560110
500. “From Metadynamics to Dynamics”
P. Tiwary and M. Parrinello
Phys. Rev. Lett., **111** (23), 230602 (2013), DOI: 10.1103/PhysRevLett.111.230602
501. “Thermodynamical Description of a Quasi-First-Order Phase Transition from the Well-Tempered Ensemble”
O. Valsson and M. Parrinello
J. Chem. Theory Comput., **9**, 5267-5276 (2013), DOI: 10.1021/ct400859f
502. “Free-energy landscape of protein oligomerization from atomistic simulations”
A. Barducci, M. Bonomi, M.K. Prakash and M. Parrinello
PNAS, **110** (49), E4708-E4713 (2013)
503. “Controlling and Predicting Crystal Shapes: The Case of Urea”
M. Salvalaglio, T. Vetter, M. Mazzotti and M. Parrinello
Anges. Chem. Int. Ed., **52**, 13369 – 13372 (2013), DOI: 10.1002/anie.201304562
504. “1,3,5-Tris(4-bromophenyl)benzeneprenucleation clusters from meta-dynamics”
M. Salvalaglio, F. Giberti and M. Parrinello
ActaCryst., C70, 132–136 (2014), DOI:10.1107/S2053229613026946
505. “Evaluating functions of positive-definite matrices using colored-noise thermostats”
M. Nava, M. Ceriotti, C. Dryzun and M. Parrinello
Phys. Rev. E, **89** (2), 023302 (2014), DOI: 10.1103/PhysRevE.89.023302
506. “Anomalous water diffusion in salt solutions”
Y. Ding, A. A. Hassanali and M. Parrinello
PNAS, **111** (9), 3310-3315 (2014), DOI: 10.1073/pnas.1400675111
507. “Aqueous solutions: state of the art in ab initio molecular dynamics”
A. A. Hassanali, J. Cuny, V. Verdolino and M. Parrinello
Phil. Trans. R. Soc. A, **372**, 20120482 (2014), DOI: 10.1098/rsta.2012.0482

508. “Assessing the Reliability of the Dynamics Reconstructed from Metadynamics”
M. Salvalaglio, P. Tiwary and M. Parrinello
J. Chem. Theory Comput., **10**, 1420-1425 (2014), DOI: 10.1021/ct500040r
509. “The role of the umbrella inversion mode in proton diffusion”
A. A. Hassanali, F. Giberti, G. C. Sosso and M. Parrinello
Chem. Phys. Lett., **599**, 133-138 (2014), DOI: 10.1016/j.cplett.2014.03.034
510. “Well-Tempered Metadynamics Converges Asymptotically”
J. F. Dama, M. Parrinello and G. A. Voth
Phys. Rev. Lett., **112**, 240602 (2014), DOI: 10.1103/PhysRevLett.112.240602
511. “Variational Approach to Enhanced Sampling and Free Energy Calculations”
O. Valsson and M. Parrinello
Phys. Rev. Lett., **113** (9), 090601 (2014), DOI: 10.1103/PhysRevLett.113.090601
512. “Transition-Tempered Metadynamics: Robust, Convergent Metadynamics via On-the Fly Transition Barrier Estimation”
J. F. Dama, G. Rotskoff, M. Parrinello and G. A. Voth
J. Chem. Theory Comput., **10**, 3626-3633 (2014), DOI: 10.1021/ct500441q
513. “G-triplex structure and formation propensity”
L. Cerofolini, J. Amato, A. Giachetti, V. Limongelli, E. Novellino, M. Parrinello, M. Fragai, A. Randazzo and C. Luchinat
Nucleic Acids Research, **42** (21), 13393-13404 (2014), DOI: 10.1093/nar/gkul1084
514. “The Role of Quantum Effects on Structural and Electronic Fluctuations in Neat and Charged Water”
F. Giberti, A. A. Hassanali, M. Ceriotti and M. Parrinello
Phys. Chem. B, **118**, 13226-13235 (2014), DOI: 10.1021/jp507752e
515. “Insight into the nucleation of urea crystals from the melt”
F. Giberti, M. Salvalaglio, M. Mazzotti and M. Parrinello
Chemical Engineering Science, **121**, 51–59 (2015), DOI: 10.1016/j.ces.2014.08.032
516. “A Time-Independent Free Energy Estimator for Metadynamics”
P. Tiwary and M. Parrinello
J. Phys. Chem. B, **119** (3), 736–742 (2015), DOI: 10.1021/jp504920s
517. “Molecular dynamics simulations of urea nucleation from aqueous solution”
M. Salvalaglio, C. Perego, F. Giberti, M. Mazzotti and M. Parrinello
PNAS, **112** (1), E6 - E14 (2015), DOI: 10.1073/pnas.1421192111
518. “Kinetics of protein-ligand unbinding: Predicting pathways, rates, and rate-limiting steps”
P. Tiwary, V. Limongelli, M. Salvalaglio and M. Parrinello
PNAS, **112** (5), E386-E391 (2015), DOI: 10.1073/pnas.1424461112
- 518a “PNAS Plus Significance Statements”
P. Tiwary, V. Limongelli, M. Salvalaglio and M. Parrinello
PNAS, **112** (5), 1256-1258 (2015), DOI: 10.1073/pnas.ss11205

519. “Energetics and Structural Characterization of the large-scale Functional Motion of Adenylate Kinase”
E. Formoso, V. Limongelli and M. Parrinello
Scientific Reports, **5**, 8425, (2015), DOI: 10.1038/srep08425
520. “Combustion Chemistry via Metadynamics: Benzyl Decomposition Revisited”
D. Polino and M. Parrinello
J. Phys. Chem. A, **119**, 978 – 989, (2015), DOI: 10.1021/jp5118807
521. “Path Integral Metadynamics”
R. Quhe, M. Nava, P. Tiwary and M. Parrinello
J. Chem. Theory Comput., **11** (4), 1383-1388 (2015) DOI: 10.1021/ct501002a
522. “Probing the Unfolded Configurations of a β -Hairpin Using Sketch-Map”
A. Ardévol, G. A. Tribello, M. Ceriotti and M Parrinello
J. Chem. Theory Comput., **11** (3), 1086-1093 (2015), DOI: 10.1021/ct500950z
523. “Metadynamics Studies of Crystal Nucleation”
F. Giberti, M. Salvalaglio and M. Parrinello
IUCrJ, **2**, 256–266 (2015), DOI: 10.1107/S2052252514027626
524. “Heterogeneous Crystallization of the Phase Change Material GeTe via Atomistic Simulations”
G. C. Sosso, M. Salvalaglio, J. Behler, M. Bernasconi and M. Parrinello
J. Phys. Chem. C, 2015, **119** (11), pp 6428–6434 DOI: 10.1021/acs.jpcc.5b00296
525. “Molecular dynamics simulations of solutions at constant chemical potential”
C. Perego, M. Salvalaglio and M. Parrinello
J. Chem. Phys., **142**, 144113 (2015), DOI: 10.1063/1.4917200
526. “Well-Tempered Variational Approach to Enhanced Sampling”
O. Valsson and Michele Parrinello
J. Chem. Theory Comput., **11**, 1996-2002 (2015), DOI: 10.1021/acs.jctc.5b00076
527. “Urea homogeneous nucleation mechanism is solvent dependent”
M. Salvalaglio, M. Mazzotti and M. Parrinello
The Royal Society of Chemistry 2015, Faraday Discuss. **179**, 291–307, (2015)
DOI: 10.1039/c4fd00235k
528. “Variationally Optimized Free-Energy Flooding for Rate Calculation”
J. McCarty, O. Valsson, P. Tiwary and M. Parrinello
Phys. Rev. Lett., **115** (7), 070601 (2015), DOI: 10.1103/PhysRevLett.115.070601
529. “de Broglie Swapping Metadynamics for Quantum and Classical Sampling”
M. Nava, R. Quhe, F. Palazzesi, P. Tiwary and M. Parrinello
J. Chem. Theory Comput., **11** (11), pp 5114–5119 (2015), DOI: 10.1021/acs.jctc.5b00818
530. “A perturbative solution to metadynamics ordinary differential equation”
P. Tiwary, J. Dama and M. Parrinello
J. Chem. Phys. **143**, 234112 (2015), DOI: 10.1063/1.4937945

531. “General Protein Data Bank-Based Collective Variables for Protein Folding”
A. Ardévol, F. Palazzesi, G. A. Tribello and M. Parrinello
J. Chem. Theory Comput., **12** (1), pp 29–35 (2016), DOI: 10.1021/acs.jctc.5b00714
532. “Enhanced, targeted sampling of high-dimensional free-energy landscapes using variationally enhanced sampling, with an application to chignolin”
P. Shaffer, O. Valsson and M. Parrinello
PNAS, **113** (5), 1150-1155 (2016), DOI: 10.1073/pnas.1519712113
533. “The interaction with gold suppresses fiber-like conformations of the amyloid β (16–22) peptide”
L. Bellucci, A. Ardévol, M. Parrinello, H. Lutz, H. Lu, T. Weidner and S. Corni
Nanoscale, **8**, 8737-8748 (2016), DOI: 10.1039/C6NR01539E
534. “Enhancing Important Fluctuations: Rare Events and Metadynamics from a Conceptual Viewpoint”
O. Valsson, P. Tiwary and M. Parrinello
Annurev. Phys. Chem., **67**, 59-184 (2016), DOI: 10.1146/annurev-physchem-040215-112229
535. “Bespoke Bias for Obtaining Free Energy Differences within Variationally Enhanced Sampling”
J. McCarty, O. Valsson and M. Parrinello
J. Chem. Theory Comput., **12** (5), pp 2162–2169 (2016), DOI: 10.1021/acs.jctc.6b00125
536. “Characterization of Vanadium Species in Mixed Chloride-Sulfate Solutions: An Ab Initio Metadynamics Study”
M. Bon, T. Laino, A. Curioni and M. Parrinello
J. Phys. Chem. C, **120** (20), pp 10791–10798 (2016), DOI: 10.1021/acs.jpcc.6b02642
537. “Dimer Metadynamics”
M. Nava, F. Palazzesi, C. Perego and M. Parrinello
arXiv:1607.04846v1, cond-mat.stat-mech (2016)
538. “Communication: Role of explicit water models in the helix folding processes”
F. Palazzesi, M. Salvalaglio, A. Barducci and M. Parrinello
J. Chem. Phys., **145**, 121101 (2016), DOI: 10.1063/1.49633040
539. “Chemical potential calculations in dense liquids using metadynamics”
C. Perego, F. Giberti and M. Parrinello
Eur. Phys. J. Special Topics, **225**, 1621-1628 (2016), DOI: 10.1140/epjst/e2016-60094-x
<http://rdcu.be/uNN> (open access link)

Books, reviewed papers and conference proceedings

1. “Structure and dynamics of simple ionic liquids”
M. Parrinello and M. P. Tosi
Riv. Nuovo Cim. **2**, 1 (1979)
2. “Static and dynamical properties of molten salts”
M. Parrinello
Physics of Modern Materials, Lect. Int. Course (1980), Meeting Date 1978, **2**, 661
Publisher: IAEA, Vienna, Austria
3. “A new molecular dynamics method for the study of crystal structure transformations”
M. Parrinello and A. Rahman
Melting, Localization and Chaos. Proc. 9th Midwest Solid State Theory Symp., Argonne, USA, 2-3 November 1981, 97.
Editor(s): Kalia, R. K.; Vashishta, P. Publisher: North-Holland, New York, NY (1982)
4. “Collective effects in solids and liquids”
A. H. March and M. Parrinello
Graduate Student Series in Physics
Publisher: Hilger, Bristol, UK (1982)
5. “Study of an F center in molten KCl”
M. Parrinello and A. Rahman
Monte Carlo Methods in Quantum Problems. Proc. NATO Advanced Research Workshop, Paris, France, 30 Nov-3 Dec 1982, 105. Editor(s): Kalos, M. H. Publisher: Reidel, Dordrecht, Netherlands (1984)
6. “Molecular-dynamics study of crystal structure transformations”
M. Parrinello
Proc. Int. Sch. Phys. 'Enrico Fermi', course XCVII. Molecular-Dynamics Simulation of Statistical-Mechanical Systems, Varenna, Italy, 23 July – 2 August 1985, 204. Editor(s): Ciccotti, G. and Hoover, W. G. Publisher: North-Holland, Amsterdam, Netherlands (1986)
7. “The fractional quantized two-dimensional Hall effect”
E. Tosatti, M. Parrinello and C. D. Chen
Proc. Int. Sch. Phys. 'Enrico Fermi', course LXXXIX. Highlights of Condensed-Matter Theory, Varenna, Italy, 28 June-16 July 1983, 453. Editor(s): Bassani, F.; Fumi, F.; Tosi, M.P. Publisher: North-Holland, Amsterdam, Netherlands (1985)
8. “Molecular dynamics at constant external stress: studies of crystal structure transformations”
M. Parrinello
Comm. Eur. Communities, EUR 9833, Comput. Simul. Phys. Metall. 1 (1986)
9. “Surface reconstruction phase transition of W(001): soft modes or not?”
Z. Wang, E. Tosatti, A. Fasolino and M. Parrinello
Il Vuoto **XVI**, 232 (1986)

10. "Density functional study of liquid and amorphous silicon"
R. Car and M. Parrinello
18th Int. Conf. Phys. Semicond., Stockholm, Sweden, 11-15 August 1986, **2**, 1165.
Editor(s): Engstrom, O. Publisher: World Scientific, Singapore (1987)
11. "Equilibrium structures and dynamical processes in microclusters"
R. Car, M. Parrinello and W. Andreoni
Springer Ser. Mater. Sci. **4** (Microclusters), 134 (1987)
12. "Structural, electronic and dynamical properties of semiconductor microclusters from *ab-initio* molecular dynamics simulations"
W. Andreoni, G. Pastore, R. Car, M. Parrinello and P. Giannozzi
19th Int. Conf. Phys. Semicond., Warsaw, Poland, 15-19 August 1988, **2**, 1759. Editor(s):
Zawadzki, W. Publisher: Pol. Acad. Sci., Inst. Phys., Warsaw, Poland (1988)
13. "High temperature diffusion of hydrogen in c-Si via ab-initio molecular dynamics"
F. Buda, G. L. Chiarotti, R. Car and M. Parrinello
Int. Conf. Phys. Semicond., Warsaw, Poland, 15-19 August 1988, **2**, 1159. Editor(s):
Zawadzki, W. Publisher: Pol. Acad. Sci., Inst. Phys., Warsaw, Poland (1988)
14. "Numerical simulation of the two dimensional Hubbard model"
S. Sorella and M. Parrinello
Interacting electrons in reduced dimensions. Editor(s): Baeriswyl, D. and Campbell, D. K.
Plenum Press, New York
NATO ASI Ser. B: Phys. **213**, 47 (1989)
15. "Hydrogen diffusion in crystalline silicon"
F. Buda, G. L. Chiarotti, R. Car and M. Parrinello
Italian-Swiss Physics Meeting, Como, Italy, 11-13 May 1989
Helv. Phys. Acta **62**, 848 (1989)
16. "The unified approach for molecular dynamics and density functional theory"
R. Car and M. Parrinello
NATO ASI Ser. **B**, 455 (1989)
17. "Properties of liquid As: a first principles calculation"
X. P. Li, P. B. Allen, R. Car and M. Parrinello
Mat. Res. Soc. Symp. Proc. **141**, 229 (1989)
18. "Ab-initio molecular dynamics studies of microclusters"
W. Andreoni, G. Pastore, R. Car, M. Parrinello and P. Giannozzi
Band Structure Engineering in Semiconductor Microstructures. Editor(s): Abram, R. A. and
Jaros, M. Plenum Press, New York
NATO ASI Ser. B **189**, 129 (1989)
19. "Ab-initio molecular dynamics simulation of alkali-metal microclusters"
W. Andreoni, P. Ballone, R. Car and M. Parrinello
Atomistic Simulation of Materials, 87. Editor(s): Vitek, V. and Srolovitz, D. J. Publisher:
Plenum Publishing Corporation (1989)

20. "Surface phonons from ab-initio molecular dynamics: Si(111)2x1"
F. Ancilotto, W. Andreoni, A. Selloni, R. Car and M. Parrinello
Proc. PHONONS '89, 3rd Int. Conf. Phonon Phys. and 6th Int. Conf. Phonon Scattering in Condensed Matter, Heidelberg, Germany, **2**, 931. Editor(s): Hunklinger, S., Weiss, G. and Ludwig, G. Publisher: World Scientific Co. Pte. Ltd., Singapore (1990)
21. "First-principles calculations of self-diffusion coefficients in silicon"
P. E. Blöchl, D. B. Laks, S. T. Pantelides, E. Smargiassi, R. Car, W. Andreoni and M. Parrinello
Proc. 20th Int. Conf. Phys. Semicond., Thessaloniki, Greece, 6-10 August 1990, **1**, 533. Editor(s): Anastassakis, E.M. and Joannopoulos, J.D. Publisher: World Scientific Publishing Co. Pte. Ltd., Singapore (1990)
22. "Theory of structure and properties of hydrogenated amorphous silicon"
G. L. Chiarotti, F. Buda, R. Car and M. Parrinello
Proc. 20th Int. Conf. Phys. Semicond., Thessaloniki, Greece, 6-10 August 1990, **3**, 2593. Editor(s): Anastassakis, E.M. and Joannopoulos, J.D. Publisher: World Scientific Publishing Co. Pte. Ltd., Singapore (1990)
23. "Input and output documentation. QMSCP from MOTECC-90"
A. Feuston, E. Clementi and M. Parrinello
MOTECC-90 "Modern Techniques in Computational Chemistry"
(IBM Corp. 1989, 1990), 586
24. "Hydrogen in crystalline and amorphous silicon"
G. L. Chiarotti, F. Buda, R. Car and M. Parrinello
Mater. Res. Soc. Symp. Proc. **163** (Impurities, Defects and Diffusion in Semiconductors: Bulk and Layered Structures), 383 (1990)
25. "*Ab initio* molecular dynamics simulation of molten KSi"
G. Galli and M. Parrinello
Liquids, Proc. 1st Liq. Matter Conf. Eur. Phys. Soc., Lyon, France, 7-11 July 1990, SA227. Editor(s): Bratos, Savo; Hansen, Jean-Pierre; Leicknam, Jean-Claude. Publisher: Hilger, Bristol, UK (1991)
26. "First-principles molecular dynamics"
M. Parrinello
Mod. Tech. Comput. Chem.: MOTECC-91, 833. Editor(s): Clementi, E. Publisher: ESCOM, Leiden, Netherlands (1991)
27. "First-principles molecular dynamics studies of diffusion processes in crystalline silicon"
G. L. Chiarotti, F. Buda, E. Smargiassi, R. Car and M. Parrinello
Proc. Electrochem. Soc. 91-4, 175 (1991)
28. "Ab-initio molecular dynamics: principles and practical implementation"
G. Galli and M. Parrinello
NATO ASI Ser., E 205 (Comput. Simul. Mater. Sci.), 283 (1991)
29. "Si(111): (2x1) reconstruction and surface phonons from *ab-initio* molecular dynamics"
F. Ancilotto, W. Andreoni, A. Selloni, R. Car and M. Parrinello
Phys. Scr. **T35**, 21 (1991)

30. “Novel semiconductors and intermetallic compounds - In search of new materials”
K. H. Vogel, R. Nesper, P. E. Blöchl and M. Parrinello
C4 Bulletin **4**, 4 (1991)
31. “Strong coupling regime in the Hubbard model at low densities”
A. Parola, S. Sorella, M. Parrinello and E. Tosatti
Dynamics of Magnetic Fluctuations in High-Temperature Superconductors. Editor(s):
Reiter, G., Horsch, P. and Psaltakis, G. P. Publisher: Plenum Press, New York
NATO ASI Ser. B: Phys. **246**, 255 (1991)
32. “Microscopic structure of amorphous covalent alloys probed by ab initio molecular
dynamics: silicon carbide”
F. Finocchi, G. Galli, M. Parrinello and C. M. Bertoni
21st Int. Conf. Phys. Semicond. **2**, 1980. Editor(s): Jiang, Ping; Zheng, Hou-Zhi. Publisher:
World Scientific, Singapore (1992)
33. “Ab initio molecular dynamics”
M. Parrinello
Proc. 13th Taniguchi Symp., Kashikojuna, Japan, 6-9 November 1990
Molecular Dynamics Simulations. Springer Ser. Solid-State Sci. **103**, 151 Editor(s):
Yonezawa, F. Publisher: Springer-Verlag, Berlin, Heidelberg (1992)
34. “Structural and electronic properties of pure and doped fullerenes”
W. Andreoni, F. Gygi and M. Parrinello
NATO ASI Ser. C **374**, 333 (1992)
35. “Properties of doped fullerenes: *ab-initio* molecular dynamics studies”
W. Andreoni and M. Parrinello
Proc. 1st Ital. Workshop on Fullerenes, Bologna, Italy, 6-7 February 1992. World Sci. Adv.
Ser. Fullerenes **2**, 191 (1992)
36. “Electronic structure optimization in plane-wave-based density functional calculations by
direct inversion in the iterative subspace”
J. Hutter, H. P. Lüthi and M. Parrinello
Comput. Mater. Sci. **2**, 244 (1994)
37. “Hydrogenated amorphous carbon from compression of acetylene and polyacetylene”
M. Bernasconi, M. Parrinello, G. L. Chiarotti, P. Focher and E. Tosatti
High Pressure Sci. Technol., Proc. Jt. Airapt XXXIII EHPRG Int. Conf. (1996), Meeting
Date 1995, 846-848
Publisher: World Scientific, Singapore
38. “Pressure induced solid-solid phase transformation via first-principle simulations”
M. Bernasconi, G. L. Chiarotti, P. Focher, S. Scandolo, E. Tosatti and M. Parrinello
22nd International Conference on the Physics of Semiconductors, Vancouver (1994)
Publisher: World Scientific, 1995, p. 193-6, vol. 1 of 3 vol.

39. “Ab initio molecular dynamics simulation of the solvation and transport of hydronium and hydroxyl ions in water”
M. Tuckerman, K. Laasonen, M. Sprik and M. Parrinello
Ultrafast Chem. Phys. Processes Mol. Syst., Lausanne Conf. (1996), Meeting Date 1995, 578-582
Publisher: World Scientific, Singapore
40. “*Ab-initio* simulation of phase transformations under pressure”
M. Bernasconi, M. Benoit, M. Parrinello, G. L. Chiarotti, P. Focher and E. Tosatti
15th General Conference of the Condensed Matter Division of the European Physical Society, Baveno-Stresa, Italy, 22-25 April 1996
Physica Scripta **T66**, 98 (1996)
Publisher: R. Swedish Acad. Sci
41. “From silicon to RNA: the coming of age of *ab initio* molecular dynamics”
M. Parrinello
Solid State Commun. **102**, 107 (1997)
42. “Simple molecular systems at very high pressures: computer simulation studies”
G. L. Chiarotti, F. Ancilotto, M. Bernasconi, S. Bernard, C. Cavazzoni, P. Focher, J. Kohanoff, M. Parrinello, S. Scandolo, S. Serra and E. Tosatti
Koatsuryoku no Kagaku to Gijutsu (1998)
Proc. Int. Conf. AIRAPT 16, Kyoto, Japan, 25-29 August 1997 and HPCJ 38, 172 (1997).
Editor(s): Nakahara, M. Publisher: Japan Society of High Pressure Science and Technology
43. “Quantum effects on phase transitions in high-pressure ice”
M. Benoit, D. Marx and M. Parrinello
Computational Modelling of Issues in Materials Science, Proc. Symp. D, ICAM/E-MRS Conf., Strasbourg, France, 16-20 June 1997. Publisher: Elsevier, Lausanne, Switzerland (1997)
Comp. Mat. Science **10**, 88 (1998)
44. “Pressure effects on hydrogen bonding in the disordered phase of solid HBR”
T. Ikeda, M. Sprik, K. Terakura and M. Parrinello
Phys. Rev. Lett. **81**, 4416 (1998)
45. “Experimental and computational studies of Si-doped fullerenes”
I. M. L. Billas, W. Branz, F. Tast, N. Malinowski, M. Heinebrodt, T. P. Martin, M. Boero, C. Massobrio and M. Parrinello
ISSPIC9, 1-5 September 1998, Lausanne, Switzerland
Eur. Phys. J. D.
46. “Ab initio simulation of chemical processes in realistic environments”
M. Parrinello
J. Mol. Struct. (Theochem) **463**, 111 (1999)
47. “Experimental and computational studies of heterofullerenes”
I. M. L. Billas, W. Branz, N. Malinowski, F. Tast, M. Heinebrodt, T. P. Martin, C. Massobrio, M. Boero and M. Parrinello
4th Int. Conf. Nanostruct. Mat. (NANO '98), Stockholm, Sweden, 14-19 June 1998
NanoStructured Materials **12**, 1071 (1999), Elsevier Science Ltd. (1999)

48. “Ziegler-Natta heterogeneous catalysis by first principles computer experiments”
M. Boero, M. Parrinello and K. Terakura
International Symposium on Surface and Interface: Properties of Different Symmetry
Crossing 98, Tokyo, Japan, 19-21 November 1998
Surf. Sci. **438**, 1 (1999)
49. “The role of quantum effects and ionic defects in high-density ice”
M. Benoit, D. Marx and M. Parrinello
9th International Conference on Solid State Protonic Conductors, Bled, Slovenia, 17-21
August 1998
Sol. State Ionics **125**, 23 (1999)
50. “Compton anisotropy from Wannier functions in the case of ice I_h”
A. H. Romero, P. L. Silvestrelli and M. Parrinello
15th Latin American Symposium on Solid State Physics
Physica Stat. Sol. **220**, 703 (2000)
51. “Car-Parrinello simulation of water at supercritical conditions”
M. Boero, K. Terakura, T. Ikeshoji, C. C. Liew and M. Parrinello
Proc. 5th Int. Conf. Comp. Phys. (Computational Physics and Related Topics), Kanazawa,
Japan, 11-13 October 1999
Progress of Theoretical Physics Supplement **138**, 259 (2000)
52. “Reactive liquids from first principles”
M. Sprik and M. Parrinello
Europhys. News **31**, 9 (2000)
53. “Simulating complex systems without adjustable parameters”
M. Parrinello
Comp. Sci. Eng. **2**, 22 (2000)
54. “Modelling photoreactions in proteins by density functional theory”
C. Molteni, I. Frank and M. Parrinello
Comp. Mat. Sci. **20**, 311 (2001)
55. “A new constant-pressure ab initio/classical molecular dynamics method: simulation of
pressure-induced amorphization in a Si₃₅H₃₆ cluster”
R. Martoňák, C. Molteni and M. Parrinello
Comp. Mat. Sci. **20**, 293 (2001)
56. “Car-Parrinello molecular dynamics investigation of active surfaces and Ti catalytic sites in
Ziegler-Natta heterogeneous catalysis”
H. Weiss, M. Boero and M. Parrinello
Proc. Macromol. Symposia **173**, 137 (2001)
57. “First principles study of active sites in Ziegler-Natta heterogeneous catalysis”, in: Micro-
kinetics and dynamics of individual active sites in catalytic reactions
M. Boero, M. Parrinello and K. Terakura
Tech. and Edu. Pubs., ed. by M. Terakura and N. Otsuka, **30** (2001)

58. “First principles simulations of hemeproteins: From the active center to the full protein”
A. Rovira and M. Parrinello
Scientific Highlight of the Month, **9**, 138 (2001)
59. “Car-Parrinello molecular dynamics investigation of active surfaces and Ti/V catalytic sites”, in: Ziegler-Natta heterogeneous catalysis in future technologies for polyolefin and olefin polymerization catalysis”
Tech. and Edu. Pubs., ed. by M. Terano and T. Shiono, **210** (2002)
60. “Die Physik des Wassers (Kurzfassung)”
M. Parrinello
Nova Acta Leopoldina **NF 85**, 97 (2002)
61. “Hydrogen storage in carbon nanotubes”
M. Becher, M. Haluska, M. Hirscher et al.
C. R. Phys. **4**, 1055 (2003)
62. “Protein folding with combined parallel tempering and metadynamics”
G. Bussi, F.L. Gervasio, A. Laio, M. Parrinello
HPC-Europa: Science and Supercomputing in Europe (2006)
Edited by P. Alberigo, G. Erbacci and F. Garofalo
63. „COMP 120-Applying network to the structure analysis and modeling of helical membrane proteins“
Author(s): Mantz, YA; Branduardi, D; Parrinello, M
Conference Information: 236th National Meeting of the American-Chemical-Society, AUG 17-21, 2008 Philadelphia PA
Abstracts of papers of the Am. Chem.Soc., **236** Meeting Abstract: 277-COMP (2008)
64. “Eppur si muove”
M. Parrinello
Book: Imperial College Press; Physical Biology: From Atoms to Medicine, Editor Ahmed E. Zewail, Chapter 11, (2009)
65. „A hybrid approach to Fermi operator expansion“
M. Ceriotti, T.D. Kuhne, M. Parrinello
Conference information: Computational Methods in Science and Engineering, Advances in Computational Science, Hersonissos, Crete Greece
AIP Conference Proceedings, 658-61, (2009)

Patents

1. “Atomic force microscope with high dynamic range using bunny or dopy balls”
J. K. Gimzewski, M. Parrinello and B. Reihl
IBM Technical Disclosure Bulletin, **35**, 410 (1992)

Research Reports

1. “Structure of hydrogenated amorphous silicon from ab-initio molecular dynamics”
F. Buda, G. L. Chiarotti, R. Car and M. Parrinello
IBM Research Division, Physics, **RZ 2156** (1991)
2. “Adiabaticity in first-principles molecular dynamics”
P. E. Blöchl and M. Parrinello
IBM Research Division, Physics, **RZ 2161** (1991)
3. “Zero point motion effects on the Structure of C₆₀”
J. Kohanoff, W. Andreoni and M. Parrinello
IBM Research Division, Physics, **RZ 2320** (1992)