Mauro Ferrario

List of Publications by Year
in descending order

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121 papers	4,326 citations	126907 33 h-index	114465 63 g-index
128 all docs	128 docs citations	128 times ranked	3086 citing authors

#	Article	IF	Citations
1	High-throughput generation of potential energy surfaces for solid interfaces. Computational Materials Science, 2022, 207, 111302.	3.0	4
2	A new boundary driven NEMD scheme for heat and particle diffusion in binary mixtures. Molecular Physics, 2021, 119, .	1.7	6
3	Monitoring water and oxygen splitting at graphene edges and folds: Insights into the lubricity of graphitic materials. Carbon, 2020, 156, 93-103.	10.3	38
4	Quantum Mechanics/Molecular Mechanics (QM/MM) applied to tribology: Real-time monitoring of tribochemical reactions of water at graphene edges. Computational Materials Science, 2020, 173, 109400.	3.0	9
5	High-throughput screening of the static friction and ideal cleavage strength of solid interfaces. Scientific Reports, 2019, 9, 17062.	3.3	15
6	Holonomic Constraints: A Case for Statistical Mechanics of Non-Hamiltonian Systems. Computation, 2018, 6, 11.	2.0	9
7	Molecular Dynamics vs. Stochastic Processes: Are We Heading Anywhere?. Entropy, 2018, 20, 348.	2.2	2
8	Ideal adhesive and shear strengths of solid interfaces: A high throughput ab initio approach. Computational Materials Science, 2018, 154, 517-529.	3.0	22
9	Thermal Diffusion in Binary Mixtures: Transient Behavior and Transport Coefficients from Equilibrium and Nonequilibrium Molecular Dynamics. Langmuir, 2017, 33, 11281-11290.	3.5	15
10	On the configurational temperature NosÃ¨â€“Hoover thermostat. Physica A: Statistical Mechanics and Its Applications, 2016, 461, 19-35.	2.6	12
11	First-Principle Molecular Dynamics of Sliding Diamond Surfaces: Tribochemical Reactions with Water and Load Effects. Journal of Low Temperature Physics, 2016, 185, 174-182.	1.4	9
12	Size-dependent commensurability and its possible role in determining the frictional behavior of adsorbed systems. Physical Chemistry Chemical Physics, 2016, 18, 28997-29004.	2.8	8
13	Non-equilibrium by molecular dynamics: a dynamical approach. Molecular Simulation, 2016, 42, 1385-1400.	2.0	30
14	On the establishment of thermal diffusion in binary Lennard-Jones liquids. European Physical Journal: Special Topics, 2016, 225, 1629-1642.	2.6	9
15	Probabilistic Derivation of Spatiotemporal Correlation Functions in the Hydrodynamic Limit. Journal of Physical Chemistry B, 2016, 120, 1996-2000.	2.6	2
16	Dynamical Non-Equilibrium Molecular Dynamics. Entropy, 2014, 16, 233-257.	2.2	41
17	Transient behavior of a model fluid under applied shear. Journal of Chemical Physics, 2013, 138, 184501.	3.0	0
18	Coarse-graining stiff bonds. European Physical Journal: Special Topics, 2011, 200, 107-129.	2.6	3

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19	Ab initio calculation of adhesion and potential corrugation of diamond (001) interfaces. Computer Physics Communications, 2011, 182, 1796-1799.	7.5	6
20	Onset of frictional slip by domain nucleation in adsorbed monolayers. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 1311-1316.	7.1	32
21	Correction for Reguzzoni et al., Onset of frictional slip by domain nucleation in adsorbed monolayers. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 5693-5693.	7.1	0
22	Ab initiostudy on the surface chemistry and nanotribological properties of passivated diamond surfaces. Physical Review B, 2009, 79, .	3.2	91
23	Boundary-lubricated friction in presence of a nano-well. Journal of Materials Science, 2008, 43, 3435-3440.	3.7	0
24	Lubricated friction on nanopatterned surfaces via molecular dynamics simulations. Physical Review B, 2008, 77, .	3.2	18
25	Potential energy surface for rare gases adsorbed on Cu(111): parameterization of the gas/metal interaction potential. Journal of Physics Condensed Matter, 2007, 19, 305008.	1.8	18
26	Pressure Induced Friction Collapse of Rare Gas Boundary Layers Sliding over Metal Surfaces. Physical Review Letters, 2007, 99, 176101.	7.8	37
27	Condensed matter theory by computer simulation: from materials to chemical biology features. Europhysics News, 2007, 38, 18-22.	0.3	0
28	Nonlinear Effects in Molecular Dynamics of the Liquid State. Advances in Chemical Physics, 2007, , 225-275.	0.3	9
29	Dynamical Properties of Hydrogen-Bonded Liquids. Advances in Chemical Physics, 2007, , 277-320.	0.3	42
30	Nonlinear mobility of a driven system: Temperature and disorder effects. Surface Science, 2007, 601, 3676-3681.	1.9	11
31	Partially folded states of HIV-1 protease: Molecular dynamics simulations and ligand binding. Computational and Theoretical Chemistry, 2006, 769, 111-121.	1.5	6
32	Introduction: Condensed Matter Theory by Computer Simulation. , 2006, , 1-11.		2
33	Molecular dynamics simulations of the Trp repressorâ€“DNA complex and the AV77 mutant. Computer Physics Communications, 2005, 169, 130-134.	7.5	1
34	Experimental and Simulative Dissociation of Dimeric Cu,Zn Superoxide Dismutase Doubly Mutated at the Intersubunit Surface. Biophysical Journal, 2005, 88, 2875-2882.	0.5	3
35	Effective Binding Force Calculation in Dimeric Proteins. Molecular Simulation, 2004, 30, 807-816.	2.0	11
36	Blue Moon Approach to Rare Events. Molecular Simulation, 2004, 30, 787-793.	2.0	69

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37	Structure of NaCl and KCl concentrated aqueous solutions byab initiomolecular dynamics. Molecular Physics, 2004, 102, 959-966.	1.7	38
38	Static and dynamic water molecules in Cu,Zn superoxide dismutase. Proteins: Structure, Function and Bioinformatics, 2003, 51, 607-615.	2.6	18
39	A Microscopic Description of Concentrated Potassium Fluoride Aqueous Solutions by Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2003, 107, 2354-2361.	2.6	24
40	Constant pressure-constant temperature molecular dynamics: a correct constrained NPT ensemble using the molecular virial. Molecular Physics, 2003, 101, 765-778.	1.7	103
41	Effective binding force calculation in a dimeric protein by molecular dynamics simulation. Journal of Chemical Physics, 2002, 116, 6329-6338.	3.0	27
42	Solubility of KF in water by molecular dynamics using the Kirkwood integration method. Journal of Chemical Physics, 2002, 117, 4947-4953.	3.0	87
43	Dynamics-Function Correlation in Cu, Zn Superoxide Dismutase: A Spectroscopic and Molecular Dynamics Simulation Study. Biophysical Journal, 2001, 80, 2556-2567.	0.5	26
44	Density Functional Study of the Photoactive Yellow Protein's Chromophore. Journal of Physical Chemistry B, 2001, 105, 4386-4391.	2.6	59
45	Non-Hamiltonian equations of motion with a conserved energy. Physical Review E, 2001, 64, 056125.	2.1	53
46	Structure of phosphorus-selenium glasses: results fromab initiomolecular dynamics simulations. Molecular Physics, 2000, 98, 701-707.	1.7	5
47	Rare events by constrained molecular dynamics. Journal of Molecular Liquids, 2000, 89, 1-18.	4.9	30
48	Reversible integrators for basic extended system molecular dynamics. Molecular Physics, 1999, 97, 825-832.	1.7	15
49	Reversible integrators for basic extended system molecular dynamics. Molecular Physics, 1999, 97, 825-832.	1.7	8
50	Interaction of Cl2 molecules with GaAs(110) surface. Surface Science, 1998, 402-404, 47-51.	1.9	2
51	Constrained and nonequilibrium molecular dynamics. , 1998, , .		1
52	Nonadiabatic molecular dynamics methods for diffusion. , 1998, , .		0
53	Long-time tails in two-dimensional fluids by molecular dynamics. Physica A: Statistical Mechanics and Its Applications, 1997, 240, 268-276.	2.6	12
54	First-principles simulation of phosphorus-selenium systems. Chemical Physics Letters, 1996, 259, 301-306.	2.6	3

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55	Molecular dynamics study of the plastic-crystalline phase transition of tetraphosphorus triselenide. Molecular Physics, 1995, 84, 727-742.	1.7	6
56	Cation transport in lithium sulphate based crystals. Molecular Physics, 1995, 86, 923-938.	1.7	25
57	SIMULATION OF CLASSICAL AND QUANTUM ACTIVATED PROCESSES IN THE CONDENSED PHASE. , 1995, , 150-190.		8
58	Simulation of superoxide-superoxide dismutase association rate for six natural variants. Comparison with the experimental catalytic rate. The Journal of Physical Chemistry, 1994, 98, 10554-10557.	2.9	28
59	Quantum effects on the solvent contribution to the activation free energy. Journal of Molecular Liquids, 1994, 61, 37-47.	4.9	5
60	Activation free energy for proton transfer in solution. Chemical Physics, 1994, 180, 181-189.	1.9	34
61	Structural fluctuations and the order-disorder phase transition in calcite. Journal of Physics Condensed Matter, 1994, 6, 1345-1358.	1.8	19
62	Dynamical behavior of the azide ion in protic solvents. Chemical Physics Letters, 1993, 213, 537-540.	2.6	50
63	Statistical geometry of hard particles on a sphere: analysis of defects at high density. Physica A: Statistical Mechanics and Its Applications, 1993, 201, 649-665.	2.6	30
64	Simulation of site-site soft-core liquid crystal models. Molecular Physics, 1993, 80, 297-312.	1.7	37
65	Scientific Visualization, a User View. , 1993, , 497-503.		0
66	Molecularâ€dynamics study of adiabatic protonâ€transfer reactions in solution. Journal of Chemical Physics, 1992, 97, 378-388.	3.0	111
67	Solvent-solute hydrogen bonding in dilute solutions of CN-and CH3CN in water and methanol. Molecular Physics, 1992, 77, 617-627.	1.7	27
68	Statistical geometry of hard particles on a sphere. Physica A: Statistical Mechanics and Its Applications, 1992, 187, 456-474.	2.6	31
69	Orientational Disorder and Structural Phase Transitions in Plastic Molecular Crystals. , 1991, , 381-393.		5
70	Activation energies by molecular dynamics with constraints. Chemical Physics Letters, 1991, 176, 581-587.	2.6	67
71	Shear-rate dependence of the viscosity of the Lennard-Jones liquid at the triple point. Physical Review A, 1991, 44, 6936-6939.	2.5	39
72	Dynamics of ion pair interconversion in a polar solvent. Journal of Chemical Physics, 1990, 93, 7137-7147.	3.0	179

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73	Molecularâ€dynamics simulation of aqueous mixtures: Methanol, acetone, and ammonia. Journal of Chemical Physics, 1990, 93, 5156-5166.	3.0	378
74	Environmental Dynamics and Electron Transfer Reactions. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1990, , 133-148.	0.2	3
75	Diffusion effects of hydrogen bond fluctuations. I. The long time regime of the translational and rotational diffusion of water. Journal of Chemical Physics, 1989, 91, 1179-1190.	3.0	55
76	Constrained molecular dynamics and the mean potential for an ion pair in a polar solvent. Chemical Physics, 1989, 129, 241-251.	1.9	234
77	A molecular dynamics study of orientational disordering in crystalline sodium nitrate. Journal of Physics Condensed Matter, 1989, 1, 6523-6542.	1.8	40
78	Molecular dynamics simulation of electron-transfer reactions in solution. The Journal of Physical Chemistry, 1989, 93, 6261-6265.	2.9	138
79	Molecular dynamics study of a sodium octanoate micelle in aqueous solution. The Journal of Physical Chemistry, 1988, 92, 819-821.	2.9	151
80	Spectroscopic and molecular dynamics studies of solvation of cyanomethane and cyanide ions. Faraday Discussions of the Chemical Society, 1988, 85, 237-253.	2.2	39
81	Molecular dynamics simulation of ion association reactions in a polar solvent. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1988, 85, 925-929.	0.2	7
82	Structure of solid tâ€butyl cyanide: A study by means of constantâ€temperature, constantâ€pressure, molecularâ€dynamics simulations. Journal of Chemical Physics, 1987, 87, 4823-4828.	3.0	8
83	Structural Transition on Cooling of Plastic Adamantane: A Molecular-Dynamics Study. Physical Review Letters, 1987, 59, 2574-2577.	7.8	18
84	Molecular-dynamics simulation of liquid methanol. The Journal of Physical Chemistry, 1987, 91, 4934-4940.	2.9	420
85	A molecular dynamics study of the rotator phase of t-butyl bromide. Journal of the Chemical Society, Faraday Transactions 2, 1987, 83, 2097.	1.1	9
86	Pair interactions and hydrogen-bond networks in models of liquid methanol. Molecular Physics, 1986, 58, 849-853.	1.7	77
87	Anion ordering in alkali cyanide crystals. Journal of Chemical Physics, 1986, 84, 3975-3985.	3.0	42
88	A molecular dynamics study of the TIP4P model of water. Chemical Physics Letters, 1985, 121, 182-186.	2.6	35
89	Constant pressure-constant temperature molecular dynamics for rigid and partially rigid molecular systems. Molecular Physics, 1985, 54, 587-603.	1.7	125
90	Structure of solid tâ€butyl cyanide: Interpretation of experimental data by means of molecular dynamics simulation. Journal of Chemical Physics, 1985, 83, 4726-4733.	3.0	7

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91	Non-linear effects in rotational dynamics in the liquid state. Molecular Physics, 1984, 53, 1251-1272.	1.7	9
92	Hydrogen bond statistics and dynamics in water: Selfâ€diffusion and dielectric relaxation. Journal of Chemical Physics, 1984, 81, 6214-6223.	3.0	19
93	A â€œmicroscopicâ€•model for the dynamics of water. Chemical Physics Letters, 1983, 98, 548-553.	2.6	9
94	Non-Gaussian effects in the computer simulation of dichloro methane. Journal of Molecular Liquids, 1983, 26, 249-260.	4.9	3
95	The structure of liquid benzene. Molecular Physics, 1983, 50, 217-227.	1.7	82
96	Molecular dynamics of rigid systems in cartesian coordinates A general formulation. Molecular Physics, 1982, 47, 1253-1264.	1.7	318
97	Computer simulation of the generalized brownian motion. Molecular Physics, 1982, 46, 875-889.	1.7	23
98	Computer simulation of dichloromethane. II. Molecular dynamics. Chemical Physics, 1982, 72, 147-154.	1.9	24
99	Dielectric relaxation as a multiplicative stochastic process. Physica A: Statistical Mechanics and Its Applications, 1982, 111, 255-272.	2.6	5
100	Molecular dynamics simulation of liquid CH2Cl2 with 3Ã—3 and 5Ã—5 site-site interactions. Advances in Molecular Relaxation and Interaction Processes, 1982, 22, 245-249.	0.5	8
101	The correlation of molecular rotational and translational kinetic energy in liquid CH2Cl2 and CHCl3. Advances in Molecular Relaxation and Interaction Processes, 1982, 23, 69-73.	0.5	5
102	Numerical solution of fokker/planck/kramers equations. Advances in Molecular Relaxation and Interaction Processes, 1982, 23, 143-178.	0.5	2
103	Computer simulation of the molecular dynamics of liquid dichloro methane. Advances in Molecular Relaxation and Interaction Processes, 1982, 24, 75-105.	0.5	8
104	Cybernetic spectroscopy of molecular rototranslation in the liquid state. Advances in Molecular Relaxation and Interaction Processes, 1982, 24, 139-148.	0.5	3
105	Molecular dynamics of CH2Cl2: temperature dependences of the far infra-red spectrum. Part 1: experimental and simulation. Advances in Molecular Relaxation and Interaction Processes, 1982, 22, 79-87.	0.5	6
106	Correlation times for liquid CH2Cl2. Advances in Molecular Relaxation and Interaction Processes, 1982, 23, 113-117.	0.5	5
107	Molecular dynamics computer simulation of liquid dichloromethane. I. Equilibrium properties. Chemical Physics, 1982, 72, 141-145.	1.9	34
108	A theory of the dielectric loss in the aligned nematic mesophase. Physica A: Statistical Mechanics and Its Applications, 1981, 108, 135-142.	2.6	1

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109	The intermolecular dimer potential of non-dipolar linear molecules. Advances in Molecular Relaxation and Interaction Processes, 1981, 20, 215-231.	0.5	5
110	Cumulant expansion of the orientational auto-correlation function. Advances in Molecular Relaxation and Interaction Processes, 1981, 19, 129-143.	0.5	3
111	Brownian motion with superimposed interaction: cosine potential and molecular dynamics simulation. Advances in Molecular Relaxation and Interaction Processes, 1981, 20, 1-10.	0.5	10
112	Intermolecular pair and trimer potentials for methyl fluoride. Advances in Molecular Relaxation and Interaction Processes, 1981, 20, 47-62.	0.5	4
113	A spectrometer for far i.r. hot broad band fluorescence in gases. Spectrochimica Acta Part A: Molecular Spectroscopy, 1981, 37, 123-127.	0.1	1
114	Itinerant oscillation with a cosine potential. Chemical Physics, 1981, 62, 481-487.	1.9	1
115	Probability diffusion in non-Markhovian, non-Gaussian molecular ensembles: A theoretical analysis and computer simulation. Zeitschrift FÃ¼r Physik B Condensed Matter and Quanta, 1981, 41, 165-176.	1.9	10
116	Role of rotational thermal bath excitation on the EPR transient regime: A theoretical discussion. Journal of Chemical Physics, 1981, 74, 235-245.	3.0	9
117	Non-gaussian distributions in computer triatomics. Chemical Physics Letters, 1980, 71, 139-144.	2.6	2
118	The mutual interaction of molecular rotation and translation. Molecular Physics, 1980, 39, 1369-1389.	1.7	19
119	Theory of transient response for arbitrarily strong driving fields. Journal of the Chemical Society, Faraday Transactions 2, 1980, 76, 542.	1.1	6
120	A generalization of the kuboâ€"freed relaxation theory. Chemical Physics Letters, 1979, 62, 100-106.	2.6	29
121	The nonâ€Markovian relaxation process as a â€˜â€˜contractionâ€™â€™ of a multidimensional one of Markovian type. Journal of Mathematical Physics, 1979, 20, 2567-2572.	1.1	67