Giovanni Ciccotti

List of Publications by Year
in descending order

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68	21,599	361413 20	98798 67
papers	citations	h-index	g-index

70	70	70	19446
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Numerical integration of the cartesian equations of motion of a system with constraints: molecular dynamics of n-alkanes. Journal of Computational Physics, 1977, 23, 327-341.	3.8	18,418
2	String method in collective variables: Minimum free energy paths and isocommittor surfaces. Journal of Chemical Physics, 2006, 125, 024106.	3.0	600
3	Molecular dynamics simulation of rigid molecules. Computer Physics Reports, 1986, 4, 346-392.	2.2	424
4	Non-Hamiltonian molecular dynamics: Generalizing Hamiltonian phase space principles to non-Hamiltonian systems. Journal of Chemical Physics, 2001, 115, 1678-1702.	3.0	273
5	?Thought-experiments? by molecular dynamics. Journal of Statistical Physics, 1979, 21, 1-22.	1.2	192
6	Blue Moon Sampling, Vectorial Reaction Coordinates, and Unbiased Constrained Dynamics. ChemPhysChem, 2005, 6, 1809-1814.	2.1	151
7	Mixed quantum-classical surface hopping dynamics. Journal of Chemical Physics, 2000, 112, 6543-6553.	3.0	141
8	Adaptive resolution molecular dynamics simulation through coupling to an internal particle reservoir. Physical Review Letters, 2012, 108, 170602.	7.8	126
9	Direct Computation of Dynamical Response by Molecular Dynamics: The Mobility of a Charged Lennard-Jones Particle. Physical Review Letters, 1975, 35, 789-792.	7.8	118
10	Introduction of Andersenâ€™s demon in the molecular dynamics of systems with constraints. Journal of Chemical Physics, 1983, 78, 7368-7374.	3.0	109
11	Solubility of KF in water by molecular dynamics using the Kirkwood integration method. Journal of Chemical Physics, 2002, 117, 4947-4953.	3.0	87
12	Methane Clathrate Hydrate Nucleation Mechanism by Advanced Molecular Simulations. Journal of Physical Chemistry C, 2014, 118, 22847-22857.	3.1	87
13	The rotation-translation coupling in diatomic molecules. Molecular Physics, 1981, 44, 979-996.	1.7	84
14	Projection of diffusions on submanifolds: Application to mean force computation. Communications on Pure and Applied Mathematics, 2008, 61, 371-408.	3.1	69
15	Clathrate structure-type recognition: Application to hydrate nucleation and crystallisation. Journal of Chemical Physics, 2015, 142, 244503.	3.0	33
16	Temperature accelerated Monte Carlo (TAMC): a method for sampling the free energy surface of non-analytical collective variables. Physical Chemistry Chemical Physics, 2011, 13, 5952.	2.8	31
17	Non-equilibrium by molecular dynamics: a dynamical approach. Molecular Simulation, 2016, 42, 1385-1400.	2.0	30
18	Mechanisms and Nucleation Rate of Methane Hydrate by Dynamical Nonequilibrium Molecular Dynamics. Journal of Physical Chemistry C, 2017, 121, 24223-24234.	3.1	30

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19	Nuclear quantum effects in electronic (non)adiabatic dynamics. European Physical Journal B, 2018, 91, 1.	1.5	28
20	Hydrodynamics from statistical mechanics: combined dynamical-NEMD and conditional sampling to relax an interface between two immiscible liquids. Physical Chemistry Chemical Physics, 2011, 13, 13177.	2.8	27
21	Nucleation of Molecular Crystals Driven by Relative Information Entropy. Journal of Chemical Theory and Computation, 2018, 14, 959-972.	5.3	27
22	A General Mechanism for Signal Propagation in the Nicotinic Acetylcholine Receptor Family. Journal of the American Chemical Society, 2019, 141, 19953-19958.	13.7	25
23	Dynamical nonequilibrium molecular dynamics reveals the structural basis for allostery and signal propagation in biomolecular systems. European Physical Journal B, 2021, 94, 144.	1.5	23
24	Molecular simulations: past, present, and future (a Topical Issue in EPJB). European Physical Journal B, 2022, 95, 1.	1.5	20
25	Time reversal symmetry in time-dependent correlation functions for systems in a constant magnetic field. Europhysics Letters, 2014, 108, 60004.	2.0	19
26	Solubility of paracetamol in ethanol by molecular dynamics using the extended Einstein crystal method and experiments. Journal of Chemical Physics, 2019, 150, 094107.	3.0	19
27	The physics of open systems for the simulation of complex molecular environments in soft matter. Soft Matter, 2019, 15, 2114-2124.	2.7	18
28	Molecular Dynamics Simulations of Nonequilibrium Phenomena and Rare Dynamical Events. , 1991, , 119-137.		17
29	Probing the Structures of Hydrated Nafion in Different Morphologies Using Temperature-Accelerated Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2013, 117, 774-782.	3.1	17
30	Exploring the Conformational Dynamics of Alanine Dipeptide in Solution Subjected to an External Electric Field: A Nonequilibrium Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2014, 10, 1376-1386.	5.3	17
31	Berni Alder and the pioneering times of molecular simulation. European Physical Journal H, 2018, 43, 303-335.	0.8	17
32	On the Equivalence of Atomic and Molecular Pressure. Journal of Physical Chemistry B, 2004, 108, 6866-6869.	2.6	16
33	Communication: Constrained molecular dynamics for polarizable models. Journal of Chemical Physics, 2018, 149, 191102.	3.0	16
34	Mass-zero constrained molecular dynamics for electrode charges in simulations of electrochemical systems. Journal of Chemical Physics, 2020, 152, 194701.	3.0	16
35	Conformational Changes in Acetylcholine Binding Protein Investigated by Temperature Accelerated Molecular Dynamics. PLoS ONE, 2014, 9, e88555.	2.5	16
36	Path integral based calculations of symmetrized time correlation functions. II. Journal of Chemical Physics, 2010, 133, 164105.	3.0	15

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37	On metastability and Markov state models for non-stationary molecular dynamics. Journal of Chemical Physics, 2016, 145, 174103.	3.0	15
38	Thermal Diffusion in Binary Mixtures: Transient Behavior and Transport Coefficients from Equilibrium and Nonequilibrium Molecular Dynamics. Langmuir, 2017, 33, 11281-11290.	3.5	15
39	Adiabatic motion and statistical mechanics via mass-zero constrained dynamics. Physical Chemistry Chemical Physics, 2020, 22, 10775-10785.	2.8	15
40	Time-reversal symmetry for systems in a constant external magnetic field. Physical Review E, 2017, 96, 012160.	2.1	14
41	Quantum Trajectories for the Dynamics in the Exact Factorization Framework: A Proof-of-Principle Test. Journal of Physical Chemistry A, 2020, 124, 6764-6777.	2.5	14
42	Modified single sweep method for reconstructing free-energy landscapes. Molecular Simulation, 2009, 35, 1116-1129.	2.0	13
43	Linearized symmetrized quantum time correlation functions calculation via phase pre-averaging. Molecular Physics, 2011, 109, 3015-3027.	1.7	13
44	Spontaneous chiral symmetry breaking in collective active motion. Physical Review E, 2016, 93, 022410.	2.1	13
45	Time reversal and symmetries of time correlation functions. Molecular Physics, 2018, 116, 3097-3103.	1.7	13
46	Combining Rare Events Techniques: Phase Change in Si Nanoparticles. Journal of Statistical Physics, 2011, 145, 812-830.	1.2	12
47	Quantum dynamical structure factor of liquid neon via a quasiclassical symmetrized method. Journal of Chemical Physics, 2013, 138, 054118.	3.0	11
48	A Structural Model of the Human Î±7 Nicotinic Receptor in an Open Conformation. PLoS ONE, 2015, 10, e0133011.	2.5	11
49	On the establishment of thermal diffusion in binary Lennard-Jones liquids. European Physical Journal: Special Topics, 2016, 225, 1629-1642.	2.6	9
50	Holonomic Constraints: A Case for Statistical Mechanics of Non-Hamiltonian Systems. Computation, 2018, 6, 11.	2.0	9
51	Electroless formation of silver nanoaggregates: an experimental and molecular dynamics approach. Molecular Physics, 2014, 112, 1375-1388.	1.7	6
52	A semi-flexible model prediction for the polymerization force exerted by a living F-actin filament on a fixed wall. Journal of Chemical Physics, 2015, 143, 145101.	3.0	6
53	The trees and the forest. European Physical Journal: Special Topics, 2015, 224, 2515-2518.	2.6	6
54	On the forceâ€“velocity relationship of a bundle of rigid bio-filaments. Journal of Chemical Physics, 2018, 148, 095101.	3.0	6

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55	A new boundary driven NEMD scheme for heat and particle diffusion in binary mixtures. Molecular Physics, 2021, 119, .	1.7	6
56	An observable for vacancy characterization and diffusion in crystals. Journal of Chemical Physics, 2013, 138, 144103.	3.0	5
57	Gas phase infrared spectra from quasi-classical Kubo time correlation functions. Molecular Physics, 2015, 113, 2894-2904.	1.7	4
58	On computing the solubility of molecular systems subject to constraints using the extended Einstein crystal method. Journal of Chemical Physics, 2019, 150, 201104.	3.0	4
59	Jarzynski on work and free energy relations: The case of variable volume. AICHE Journal, 2021, 67, .	3.6	4
60	Gas phase infrared spectra via the phase integration quasi-classical method. Molecular Simulation, 2014, 40, 196-207.	2.0	3
61	On the properties of a bundle of flexible actin filaments in an optical trap. Journal of Chemical Physics, 2016, 144, 245102.	3.0	3
62	Mass-Zero constrained dynamics and statistics for the shell model in magnetic field. European Physical Journal B, 2021, 94, 1.	1.5	3
63	Approximating Time-Dependent Quantum Statistical Properties. Entropy, 2014, 16, 86-109.	2.2	2
64	Molecular Dynamics vs. Stochastic Processes: Are We Heading Anywhere?. Entropy, 2018, 20, 348.	2.2	2
65	Jarzynski equality on work and free energy: Crystal indentation as a case study. Journal of Chemical Physics, 2022, 156, 114118.	3.0	2
66	Particle-Based Modeling of Living Actin Filaments in an Optical Trap. Polymers, 2016, 8, 343.	4.5	1
67	Ab initio accelerated molecular dynamics study of the hydride ligands in the ruthenium complex: Ru(H2)2H2(P(C5H9)3)2. Physical Chemistry Chemical Physics, 2019, 21, 25247-25257.	2.8	1
68	The breakthrough of a quantum chemist by classical dynamics: Martin Karplus and the birth of computer simulations of chemical reactions. European Physical Journal H, 2021, 46, 1.	0.8	1