Giovanni Ciccotti

List of Publications by Year in Descending Order

77 papers	21,925 citations	31 h-index	77 g-index
77 ext. papers	23,921 ext. citations	3.1 avg, IF	6.38 L-index

#	Paper	IF	Citations
77	Dynamical nonequilibrium molecular dynamics reveals the structural basis for allostery and signal propagation in biomolecular systems. *European Physical Journal B*, **2021**, 94, 144	1.2	5
76	Computer Meets Theoretical Physics. *The Frontiers Collection*, **2020**,	0.3	8
75	Adiabatic motion and statistical mechanics via mass-zero constrained dynamics. *Physical Chemistry Chemical Physics*, **2020**, 22, 10775-10785	3.6	5
74	Nucleation of Molecular Crystals Driven by Relative Information Entropy. *Journal of Chemical Theory and Computation*, **2018**, 14, 959-972	6.4	19
73	Holonomic Constraints: A Case for Statistical Mechanics of Non-Hamiltonian Systems. *Computation*, **2018**, 6, 11	2.2	7
72	Nuclear quantum effects in electronic (non)adiabatic dynamics. *European Physical Journal B*, **2018**, 91, 1	1.2	21
71	Communication: Constrained molecular dynamics for polarizable models. *Journal of Chemical Physics*, **2018**, 149, 191102	3.9	8
70	Mechanisms and Nucleation Rate of Methane Hydrate by Dynamical Nonequilibrium Molecular Dynamics. *Journal of Physical Chemistry C*, **2017**, 121, 24223-24234	3.8	21
69	Non-equilibrium by molecular dynamics: a dynamical approach. *Molecular Simulation*, **2016**, 42, 1385-1402		17
68	Probabilistic Derivation of Spatiotemporal Correlation Functions in the Hydrodynamic Limit. *Journal of Physical Chemistry B*, **2016**, 120, 1996-2000	3.4	2
67	Particle-Based Modeling of Living Actin Filaments in an Optical Trap. *Polymers*, **2016**, 8,	4.5	1
66	A Structural Model of the Human α7 Nicotinic Receptor in an Open Conformation. *PLoS ONE*, **2015**, 10, e0133011	3.7	10
65	Temperature-accelerated molecular dynamics gives insights into globular conformations sampled in the free state of the AC catalytic domain. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 2483-96	4.2	12
64	Approximating Time-Dependent Quantum Statistical Properties. *Entropy*, **2014**, 16, 86-109	2.8	2
63	Dynamical Non-Equilibrium Molecular Dynamics. *Entropy*, **2014**, 16, 233-257	2.8	33
62	Quantum dynamical structure factor of liquid neon via a quasiclassical symmetrized method. *Journal of Chemical Physics*, **2013**, 138, 054118	3.9	11
61	Multiphoton absorption of myoglobin-nitric oxide complex: relaxation by D-NEMD of a stationary state. *Journal of Physical Chemistry B*, **2012**, 116, 3397-410	3.4	10

60	Silver self aggregation in a nanodevice for enhanced Raman spectroscopy: experiments vs. simplified modeling via molecular dynamics. *Nanoscale*, **2012**, 4, 2362-71	7.7	7
59	Temperature accelerated Monte Carlo (TAMC): a method for sampling the free energy surface of non-analytical collective variables. *Physical Chemistry Chemical Physics*, **2011**, 13, 5952-9	3.6	28
58	Short range hydrogen diffusion in Na3AlH6. *Physical Chemistry Chemical Physics*, **2011**, 13, 10546-55	3.6	6
57	Combining Rare Events Techniques: Phase Change in Si Nanoparticles. *Journal of Statistical Physics*, **2011**, 145, 812-830	1.5	10
56	Direct observation of the substitution effects on the hydrogen bridge dynamics in selected Schiff bases--a comparative molecular dynamics study. *Journal of Chemical Physics*, **2011**, 134, 034308	3.9	9
55	Communications: On the linear response of mechanical systems with constraints. *Journal of Chemical Physics*, **2010**, 132, 111103	3.9	7
54	Mapping the network of pathways of CO diffusion in myoglobin. *Journal of the American Chemical Society*, **2010**, 132, 1010-7	16.4	91
53	Hydration structure of the quaternary ammonium cations. *Journal of Physical Chemistry B*, **2010**, 114, 15018-28	3.4	29
52	Linearization approximations and Liouville quantum□lassical dynamics. *Chemical Physics Letters*, **2010**, 484, 399-404	2.5	34
51	Fast simulation of polymer chains. *Journal of Chemical Physics*, **2009**, 130, 144101	3.9	3
50	Do We Have a Consistent Non-Adiabatic Quantum-Classical Statistical Mechanics?. *Springer Series in Chemical Physics*, **2009**, 437-467	0.3	
49	Bulk viscosity of the Lennard-Jones system at the triple point by dynamical nonequilibrium molecular dynamics. *Physical Review E*, **2008**, 78, 021204	2.4	14
48	Trotter-based simulation of quantum-classical dynamics. *Journal of Physical Chemistry B*, **2008**, 112, 424-32	3.4	88
47	Calculations of free energy barriers for local mechanisms of hydrogen diffusion in alanates. *Lecture Notes in Computational Science and Engineering*, **2008**, 187-206	0.3	3
46	On the assumptions underlying milestoning. *Journal of Chemical Physics*, **2008**, 129, 174102	3.9	138
45	Projection of diffusions on submanifolds: Application to mean force computation. *Communications on Pure and Applied Mathematics*, **2008**, 61, 371-408	2.5	53
44	Calculations of free energy barriers for local mechanisms of hydrogen diffusion in alanates. *Scientific Modeling and Simulation SMNS*, **2008**, 15, 187-206		21
43	Computing the acidity of liquids via ab initio molecular dynamics. *ChemPhysChem*, **2007**, 8, 2072-6	3.2	8

42	String method in collective variables: minimum free energy paths and isocommittor surfaces. *Journal of Chemical Physics*, **2006**, 125, 24106	3.9	519
41	Second-order integrators for Langevin equations with holonomic constraints. *Chemical Physics Letters*, **2006**, 429, 310-316	2.5	130
40	Blue moon sampling, vectorial reaction coordinates, and unbiased constrained dynamics. *ChemPhysChem*, **2005**, 6, 1809-14	3.2	132
39	Molecular dynamics: An account of its evolution **2005**, 425-441		2
38	Non-Equilibrium Molecular Dynamics **2005**, 745-761		7
37	Simulating Reactions That Occur Once in a Blue Moon **2005**, 1597-1611		1
36	Non-Equilibrium Molecular Dynamics **2005**, 745-761		
35	Simulating Reactions That Occur Once in a Blue Moon **2005**, 1597-1611		
34	Atomic mean-square displacements in proteins by molecular dynamics: a case for analysis of variance. *Biophysical Journal*, **2004**, 86, 2765-72	2.9	16
33	Deterministic and stochastic algorithms for mechanical systems under constraints. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2004**, 362, 1583-94	3	11
32	Algorithms for Brownian dynamics. *Molecular Physics*, **2003**, 101, 1927-1931	1.7	61
31	Constant pressure-constant temperature molecular dynamics: a correct constrained NPT ensemble using the molecular virial. *Molecular Physics*, **2003**, 101, 765-778	1.7	56
30	Constrained reaction coordinate dynamics for systems with constraints. *Molecular Physics*, **2003**, 101, 2885-2894	1.7	29
29	Surface-hopping dynamics of a spin-boson system. *Journal of Chemical Physics*, **2002**, 116, 2346-2353	3.9	83
28	Protein□trehalose□water structures in trehalose coated carboxy-myoglobin. *Journal of Chemical Physics*, **2002**, 117, 9862-9866	3.9	102
27	Effective binding force calculation in a dimeric protein by molecular dynamics simulation. *Journal of Chemical Physics*, **2002**, 116, 6329-6338	3.9	26
26	Sequential short-time propagation of quantum□classical dynamics. *Journal of Physics Condensed Matter*, **2002**, 14, 9069-9076	1.8	67
25	Solubility of KF in water by molecular dynamics using the Kirkwood integration method. *Journal of Chemical Physics*, **2002**, 117, 4947-4953	3.9	81

24	A Statistical Mechanical Theory of Quantum Dynamics in Classical Environments. *Lecture Notes in Physics*, **2002**, 445-472	0.8	16
23	Statistical mechanics of quantum-classical systems. *Journal of Chemical Physics*, **2001**, 115, 5805-5815	3.9	110
22	Non-Hamiltonian molecular dynamics: Generalizing Hamiltonian phase space principles to non-Hamiltonian systems. *Journal of Chemical Physics*, **2001**, 115, 1678-1702	3.9	244
21	Molecular dynamics simulation of carboxy-myoglobin embedded in a trehalose-water matrix. *Biophysical Journal*, **2001**, 80, 931-8	2.9	86
20	Constrained Isothermal□Isobaric Molecular Dynamics with Full Atomic Virial□ *Journal of Physical Chemistry B*, **2001**, 105, 6710-6715	3.4	13
19	Mixed quantum-classical surface hopping dynamics. *Journal of Chemical Physics*, **2000**, 112, 6543-6553	3.9	134
18	Mixed quantum-classical dynamics. *Journal of Chemical Physics*, **1999**, 110, 8919-8929	3.9	520
17	Free energy from constrained molecular dynamics. *Journal of Chemical Physics*, **1998**, 109, 7737-7744	3.9	633
16	Structural and dynamic properties of the homodimeric hemoglobin from Scapharca inaequivalvis Thr-72-->Ile mutant: molecular dynamics simulation, low temperature visible absorption spectroscopy, and resonance Raman spectroscopy studies. *Biophysical Journal*, **1998**, 75, 2489-503	2.9	6
15	Molecular dynamics study of solvation effects on acid dissociation in aprotic media. *Journal of Chemical Physics*, **1996**, 104, 6560-6568	3.9	15
14	Molecular dynamics study of a monomeric heme undecapeptide of cytochromec. *Journal of Computer-Aided Materials Design*, **1995**, 2, 9-22		3
13	Quantum effects on the solvent contribution to the activation free energy. *Journal of Molecular Liquids*, **1994**, 61, 37-47	6	5
12	Activation free energy for proton transfer in solution. *Chemical Physics*, **1994**, 180, 181-189	2.3	31
11	Hoover NPT dynamics for systems varying in shape and size. *Molecular Physics*, **1993**, 78, 533-544	1.7	871
10	Temperature and temperature control in nonequilibrium-molecular-dynamics simulations of the shear flow of dense liquids. *Physical Review A*, **1992**, 45, 3859-3866	2.6	57
9	Molecular-dynamics study of adiabatic proton-transfer reactions in solution. *Journal of Chemical Physics*, **1992**, 97, 378-388	3.9	99
8	Activation energies by molecular dynamics with constraints. *Chemical Physics Letters*, **1991**, 176, 581-587	2.5	64
7	Dynamics of ion pair interconversion in a polar solvent. *Journal of Chemical Physics*, **1990**, 93, 7137-7147	3.9	166

6	Environmental Dynamics and Electron Transfer Reactions. *Jerusalem Symposia on Quantum Chemistry and Biochemistry*, **1990**, 133-148		3
5	Constrained reaction coordinate dynamics for the simulation of rare events. *Chemical Physics Letters*, **1989**, 156, 472-477	2.5	726
4	Constrained molecular dynamics and the mean potential for an ion pair in a polar solvent. *Chemical Physics*, **1989**, 129, 241-251	2.3	221
3	Stationary nonequilibrium states by molecular dynamics. II. Newton's law. *Physical Review A*, **1984**, 29, 916-925	2.6	99
2	Stationary nonequilibrium states by molecular dynamics. Fourier's law. *Physical Review A*, **1982**, 25, 2778-2787	2.6	171
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	4.1	15568