David L Freeman

List of Publications by Year
in descending order

64 papers	2,624 citations	186209 28 h-index	189801 50 g-index
65 all docs	65 docs citations	65 times ranked	1069 citing authors

#	Article	IF	Citations
1	Elephantâ€™s Toothpaste Used as a Qualitative Demonstration of Rate versus Temperature. Journal of Chemical Education, 2020, 97, 1061-1067.	1.1	4
2	A(nother) Modification of the Ammonia Fountain Demonstration. Journal of Chemical Education, 2017, 94, 1397-1398.	1.1	0
3	Rare-event sampling: Occupation-based performance measures for parallel tempering and infinite swapping Monte Carlo methods. Journal of Chemical Physics, 2012, 137, 204112.	1.2	19
4	Numerical Investigation of the Cumulant Expansion for Fourier Path Integrals. Lecture Notes in Computer Science, 2012, , 13-22.	1.0	0
5	Monte Carlo Investigation of the Thermodynamic Properties of (H₂O)_n and (H₂O)_nH₂ (n = 2â^’20) Clusters. Journal of Physical Chemistry B, 2011, 115, 4725-4744.	1.2	12
6	Proton disorder and the dielectric constant of type II clathrate hydrates. Journal of Chemical Physics, 2010, 132, 054509.	1.2	18
7	Convergence characteristics of the cumulant expansion for Fourier path integrals. Physical Review E, 2010, 81, 066707.	0.8	3
8	The thermodynamic and ground state properties of the TIP4P water octamer. Journal of Chemical Physics, 2009, 131, 184508.	1.2	30
9	A numerical study of the asymptotic convergence characteristics of partial averaged and reweighted Fourier path integral methods. International Journal of Quantum Chemistry, 2009, 109, 2916-2925.	1.0	5
10	A stereographic projection path integral study of the coupling between the orientation and the bending degrees of freedom of water. Journal of Chemical Physics, 2008, 128, 204107.	1.2	16
11	MD simulations using distributed multipole electrostatics: Structural and spectroscopic properties of CO- and methane-containing clathrates. Molecular Physics, 2008, 106, 1675-1684.	0.8	18
12	The Quantum Mechanics of Clusters. Advances in Chemical Physics, 2007, , 139-179.	0.3	40
13	Equilibrium and Dynamical Fourier Path Integral Methods. Advances in Chemical Physics, 2007, , 61-127.	0.3	165
14	Combining smart darting with parallel tempering using Eckart space: Application to Lennardâ€“Jones clusters. Journal of Chemical Physics, 2005, 122, 114113.	1.2	12
15	Pressure dependent study of the solid-solid phase change in 38-atom Lennard-Jones cluster. Journal of Chemical Physics, 2005, 122, 094716.	1.2	12
16	Phase changes in selected Lennard-Jones X13â^’nYn clusters. Journal of Chemical Physics, 2004, 121, 856-867.	1.2	41
17	On the encapsulation of nickel clusters by molecular nitrogen. Journal of Chemical Physics, 2004, 121, 475.	1.2	5
18	Taming the rugged landscape: Production, reordering, and stabilization of selected cluster inherent structures in the X13â^’nYn system. Journal of Chemical Physics, 2004, 121, 847-855.	1.2	16

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19	Energy estimators for random series path-integral methods. Journal of Chemical Physics, 2003, 119, 10475-10488.	1.2	24
20	Heat capacity estimators for random series path-integral methods by finite-difference schemes. Journal of Chemical Physics, 2003, 119, 12119-12128.	1.2	57
21	Taming the rugged landscape: Techniques for the production, reordering, and stabilization of selected cluster inherent structures. Journal of Chemical Physics, 2003, 118, 7321.	1.2	10
22	Monte Carlo Method for Real-Time Path Integration. AIP Conference Proceedings, 2003, , .	0.3	0
23	Computational Techniques and Strategies for Monte Carlo Thermodynamic Calculations, with Applications to Nanoclusters. Reviews in Computational Chemistry, 2003, , 1-41.	1.5	9
24	Stationary tempering and the complex quadrature problem. Journal of Chemical Physics, 2002, 116, 3509-3520.	1.2	7
25	Wavelet formulation of path integral Monte Carlo. Journal of Chemical Physics, 2002, 117, 5971-5977.	1.2	11
26	Self-adaptive quadrature and numerical path integration. Journal of Chemical Physics, 2000, 113, 2522-2529.	1.2	2
27	A heat capacity estimator for Fourier path integral simulations. Journal of Chemical Physics, 2000, 112, 3990-3996.	1.2	41
28	Phase changes in 38-atom Lennard-Jones clusters. I. A parallel tempering study in the canonical ensemble. Journal of Chemical Physics, 2000, 112, 10340-10349.	1.2	240
29	Phase changes in 38-atom Lennard-Jones clusters. II. A parallel tempering study of equilibrium and dynamic properties in the molecular dynamics and microcanonical ensembles. Journal of Chemical Physics, 2000, 112, 10350-10357.	1.2	183
30	Asymptotic convergence rates of Fourier path integral methods. Journal of Chemical Physics, 1999, 110, 6657-6672.	1.2	40
31	Comment on â€œA comparison of the efficiency of Fourier- and discrete time-path integral Monte Carloâ€• [J. Chem. Phys.109, 2123 (1998)]. Journal of Chemical Physics, 1999, 111, 7685-7686.	1.2	18
32	Equilibrium and Dynamical Path Integral Methods. , 1999, , 213-245.		1
33	The melting transition of Ni7 and Ni7H as modeled by a semi-empirical potential. Chemical Physics Letters, 1998, 295, 366-372.	1.2	7
34	A semi-empirical potential for simulations of transition metal clusters: Minima and isomers of Nin (n=2â€“13) and their hydrides. Journal of Chemical Physics, 1998, 108, 729-742.	1.2	66
35	Dynamic path integral methods: A maximum entropy approach based on the combined use of real and imaginary time quantum Monte Carlo data. Journal of Chemical Physics, 1998, 108, 3871-3875.	1.2	28
36	Theoretical studies of the effect of hydrogenâ€“hydrogen interactions on the structural and dynamical properties of metal/hydrogen clusters. Journal of Chemical Physics, 1998, 108, 4031-4038.	1.2	16

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37	A j-walking algorithm for microcanonical simulations: Applications to Lennard-Jones clusters. Journal of Chemical Physics, 1998, 109, 1643-1647.	1.2	21
38	MONTE CARLO METHODS IN CHEMISTRY: A TUTORIAL. , 1998, , 529-579.		0
39	COMPUTATIONAL STUDIES OF CLUSTERS:Methods and Results. Annual Review of Physical Chemistry, 1996, 47, 43-80.	4.8	70
40	Theoretical studies of the structure and dynamics of metal/hydrogen systems: Diffusion and path integral Monte Carlo investigations of nickel and palladium clusters. Journal of Chemical Physics, 1996, 105, 9686-9694.	1.2	21
41	Computational study of the structures and thermodynamic properties of ammonium chloride clusters using a parallel jumpâ€walking approach. Journal of Chemical Physics, 1996, 104, 8690-8702.	1.2	41
42	Fourier path integral Monte Carlo method for the calculation of the microcanonical density of states. Journal of Chemical Physics, 1994, 101, 848-849.	1.2	9
43	A study of low temperature heat capacity anomalies in bimetallic alloy clusters using Jâ€walking Monte Carlo methods. Journal of Chemical Physics, 1993, 98, 1428-1435.	1.2	46
44	Gibbs freeâ€energy changes for the growth of argon clusters adsorbed on graphite. Journal of Chemical Physics, 1992, 97, 4445-4452.	1.2	22
45	A dynamical definition of atomic clusters. Journal of Chemical Physics, 1991, 95, 3022-3023.	1.2	8
46	The quantum mechanics of clusters: The lowâ€temperature equilibrium and dynamical behavior of rareâ€gas systems. Journal of Chemical Physics, 1991, 95, 6658-6667.	1.2	32
47	The quantum mechanics of cluster melting. Journal of Chemical Physics, 1989, 90, 5651-5656.	1.2	66
48	Locating stationary paths in functional integrals: An optimization method utilizing the stationary phase Monte Carlo sampling function. Journal of Chemical Physics, 1989, 90, 3181-3191.	1.2	44
49	Monte Carlo studies of hydrogen fluoride clusters: Cluster size distributions in hydrogen fluoride vapor. Journal of Chemical Physics, 1989, 91, 2489-2497.	1.2	49
50	Theoretical studies of the energetics and structures of atomic clusters. Journal of Chemical Physics, 1989, 91, 612-619.	1.2	116
51	Cumulant methods and short time propagators. Journal of Chemical Physics, 1989, 91, 4242-4248.	1.2	43
52	Classical monte carlo dynamics: A simulated annealing approach to the construction of double-ended classical trajectories. International Journal of Quantum Chemistry, 1989, 36, 73-78.	1.0	3
53	Quantum Monte Carlo dynamics: The stationary phase Monte Carlo path integral calculation of finite temperature time correlation functions. Journal of Chemical Physics, 1988, 89, 5753-5763.	1.2	76
54	Partial averaging approach to Fourier coefficient path integration. Journal of Chemical Physics, 1986, 85, 4567-4583.	1.2	120

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55	Fourier path-integral Monte Carlo methods: Partial averaging. Physical Review Letters, 1985, 55, 1-4.	2.9	121
56	A comparison of energy estimators used in quantum Monte Carlo calculations. Journal of Chemical Physics, 1985, 83, 768-771.	1.2	5
57	Quantum Monte Carlo study of the thermodynamic properties of argon clusters: The homogeneous nucleation of argon in argon vapor and â€˜â€˜magic numberâ€™â€™ distributions in argon vapor. Journal of Chemical Physics, 1985, 82, 462-471.	1.2	95
58	A Monte Carlo method for quantum Boltzmann statistical mechanics. Journal of Chemical Physics, 1984, 80, 2239-2240.	1.2	67
59	A Monte Carlo method for quantum Boltzmann statistical mechanics using Fourier representations of path integrals. Journal of Chemical Physics, 1984, 80, 5709-5718.	1.2	80
60	A monte-carlo/molecular dynamics study of the diffusional recombination kinetics of C(a) + O(a) â†’ CO(g) on Pt(111). Surface Science, 1983, 134, 769-776.	0.8	30
61	Langevin analysis of the diffusion model for surface chemical reactions. Journal of Chemical Physics, 1983, 79, 2343-2350.	1.2	28
62	The influence of diffusion on surface reaction kinetics. Journal of Chemical Physics, 1983, 78, 6002-6009.	1.2	82
63	A numerical solution to the integral equation for atomic pair energies. Molecular Physics, 1978, 36, 655-667.	0.8	0
64	Coupled-cluster expansion applied to the electron gas: Inclusion of ring and exchange effects. Physical Review B, 1977, 15, 5512-5521.	1.1	153