

# David L Freeman

## List of Publications by Year in descending order

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64  
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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	Phase changes in 38-atom Lennard-Jones clusters. I. A parallel tempering study in the canonical ensemble. <i>Journal of Chemical Physics</i> , 2000, 112, 10340-10349.	1.2	240
2	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. <i>Journal of Chemical Physics</i> , 2000, 112, 10350-10357.	1.2	183
3	Equilibrium and Dynamical Fourier Path Integral Methods. <i>Advances in Chemical Physics</i> , 2007, , 61-127.	0.3	165
4	Coupled-cluster expansion applied to the electron gas: Inclusion of ring and exchange effects. <i>Physical Review B</i> , 1977, 15, 5512-5521.	1.1	153
5	Fourier path-integral Monte Carlo methods: Partial averaging. <i>Physical Review Letters</i> , 1985, 55, 1-4.	2.9	121
6	Partial averaging approach to Fourier coefficient path integration. <i>Journal of Chemical Physics</i> , 1986, 85, 4567-4583.	1.2	120
7	Theoretical studies of the energetics and structures of atomic clusters. <i>Journal of Chemical Physics</i> , 1989, 91, 612-619.	1.2	116
8	Quantum Monte Carlo study of the thermodynamic properties of argon clusters: The homogeneous nucleation of argon in argon vapor and "magic number" distributions in argon vapor. <i>Journal of Chemical Physics</i> , 1985, 82, 462-471.	1.2	95
9	The influence of diffusion on surface reaction kinetics. <i>Journal of Chemical Physics</i> , 1983, 78, 6002-6009.	1.2	82
10	A Monte Carlo method for quantum Boltzmann statistical mechanics using Fourier representations of path integrals. <i>Journal of Chemical Physics</i> , 1984, 80, 5709-5718.	1.2	80
11	Quantum Monte Carlo dynamics: The stationary phase Monte Carlo path integral calculation of finite temperature time correlation functions. <i>Journal of Chemical Physics</i> , 1988, 89, 5753-5763.	1.2	76
12	COMPUTATIONAL STUDIES OF CLUSTERS: Methods and Results. <i>Annual Review of Physical Chemistry</i> , 1996, 47, 43-80.	4.8	70
13	A Monte Carlo method for quantum Boltzmann statistical mechanics. <i>Journal of Chemical Physics</i> , 1984, 80, 2239-2240.	1.2	67
14	The quantum mechanics of cluster melting. <i>Journal of Chemical Physics</i> , 1989, 90, 5651-5656.	1.2	66
15	A semi-empirical potential for simulations of transition metal clusters: Minima and isomers of $N_{in}$ ( $n=2-13$ ) and their hydrides. <i>Journal of Chemical Physics</i> , 1998, 108, 729-742.	1.2	66
16	Heat capacity estimators for random series path-integral methods by finite-difference schemes. <i>Journal of Chemical Physics</i> , 2003, 119, 12119-12128.	1.2	57
17	Monte Carlo studies of hydrogen fluoride clusters: Cluster size distributions in hydrogen fluoride vapor. <i>Journal of Chemical Physics</i> , 1989, 91, 2489-2497.	1.2	49
18	A study of low temperature heat capacity anomalies in bimetallic alloy clusters using "walking" Monte Carlo methods. <i>Journal of Chemical Physics</i> , 1993, 98, 1428-1435.	1.2	46

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19	Locating stationary paths in functional integrals: An optimization method utilizing the stationary phase Monte Carlo sampling function. <i>Journal of Chemical Physics</i> , 1989, 90, 3181-3191.	1.2	44
20	Cumulant methods and short time propagators. <i>Journal of Chemical Physics</i> , 1989, 91, 4242-4248.	1.2	43
21	Computational study of the structures and thermodynamic properties of ammonium chloride clusters using a parallel jump-walking approach. <i>Journal of Chemical Physics</i> , 1996, 104, 8690-8702.	1.2	41
22	A heat capacity estimator for Fourier path integral simulations. <i>Journal of Chemical Physics</i> , 2000, 112, 3990-3996.	1.2	41
23	Phase changes in selected Lennard-Jones $X_{13}Y_n$ clusters. <i>Journal of Chemical Physics</i> , 2004, 121, 856-867.	1.2	41
24	Asymptotic convergence rates of Fourier path integral methods. <i>Journal of Chemical Physics</i> , 1999, 110, 6657-6672.	1.2	40
25	The Quantum Mechanics of Clusters. <i>Advances in Chemical Physics</i> , 2007, , 139-179.	0.3	40
26	The quantum mechanics of clusters: The low-temperature equilibrium and dynamical behavior of rare-gas systems. <i>Journal of Chemical Physics</i> , 1991, 95, 6658-6667.	1.2	32
27	A monte-carlo/molecular dynamics study of the diffusional recombination kinetics of $C(a) + O(a) \rightarrow CO(g)$ on Pt(111). <i>Surface Science</i> , 1983, 134, 769-776.	0.8	30
28	The thermodynamic and ground state properties of the TIP4P water octamer. <i>Journal of Chemical Physics</i> , 2009, 131, 184508.	1.2	30
29	Langevin analysis of the diffusion model for surface chemical reactions. <i>Journal of Chemical Physics</i> , 1983, 79, 2343-2350.	1.2	28
30	Dynamic path integral methods: A maximum entropy approach based on the combined use of real and imaginary time quantum Monte Carlo data. <i>Journal of Chemical Physics</i> , 1998, 108, 3871-3875.	1.2	28
31	Energy estimators for random series path-integral methods. <i>Journal of Chemical Physics</i> , 2003, 119, 10475-10488.	1.2	24
32	Gibbs free-energy changes for the growth of argon clusters adsorbed on graphite. <i>Journal of Chemical Physics</i> , 1992, 97, 4445-4452.	1.2	22
33	Theoretical studies of the structure and dynamics of metal/hydrogen systems: Diffusion and path integral Monte Carlo investigations of nickel and palladium clusters. <i>Journal of Chemical Physics</i> , 1996, 105, 9686-9694.	1.2	21
34	A j-walking algorithm for microcanonical simulations: Applications to Lennard-Jones clusters. <i>Journal of Chemical Physics</i> , 1998, 109, 1643-1647.	1.2	21
35	Rare-event sampling: Occupation-based performance measures for parallel tempering and infinite swapping Monte Carlo methods. <i>Journal of Chemical Physics</i> , 2012, 137, 204112.	1.2	19
36	Comment on "A comparison of the efficiency of Fourier- and discrete time-path integral Monte Carlo" [J. Chem. Phys. 109, 2123 (1998)]. <i>Journal of Chemical Physics</i> , 1999, 111, 7685-7686.	1.2	18

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37	MD simulations using distributed multipole electrostatics: Structural and spectroscopic properties of CO- and methane-containing clathrates. <i>Molecular Physics</i> , 2008, 106, 1675-1684.	0.8	18
38	Proton disorder and the dielectric constant of type II clathrate hydrates. <i>Journal of Chemical Physics</i> , 2010, 132, 054509.	1.2	18
39	Theoretical studies of the effect of hydrogen-hydrogen interactions on the structural and dynamical properties of metal/hydrogen clusters. <i>Journal of Chemical Physics</i> , 1998, 108, 4031-4038.	1.2	16
40	Taming the rugged landscape: Production, reordering, and stabilization of selected cluster inherent structures in the X13 <sup>n</sup> system. <i>Journal of Chemical Physics</i> , 2004, 121, 847-855.	1.2	16
41	A stereographic projection path integral study of the coupling between the orientation and the bending degrees of freedom of water. <i>Journal of Chemical Physics</i> , 2008, 128, 204107.	1.2	16
42	Combining smart darting with parallel tempering using Eckart space: Application to Lennard-Jones clusters. <i>Journal of Chemical Physics</i> , 2005, 122, 114113.	1.2	12
43	Pressure dependent study of the solid-solid phase change in 38-atom Lennard-Jones cluster. <i>Journal of Chemical Physics</i> , 2005, 122, 094716.	1.2	12
44	Monte Carlo Investigation of the Thermodynamic Properties of (H <sub>2</sub> O) <sub>n</sub> and (H <sub>2</sub> O) <sub>n</sub> H <sub>2</sub> ( <i>n</i> = 2-20) Clusters. <i>Journal of Physical Chemistry B</i> , 2011, 115, 4725-4744.	1.2	12
45	Wavelet formulation of path integral Monte Carlo. <i>Journal of Chemical Physics</i> , 2002, 117, 5971-5977.	1.2	11
46	Taming the rugged landscape: Techniques for the production, reordering, and stabilization of selected cluster inherent structures. <i>Journal of Chemical Physics</i> , 2003, 118, 7321.	1.2	10
47	Fourier path integral Monte Carlo method for the calculation of the microcanonical density of states. <i>Journal of Chemical Physics</i> , 1994, 101, 848-849.	1.2	9
48	Computational Techniques and Strategies for Monte Carlo Thermodynamic Calculations, with Applications to Nanoclusters. <i>Reviews in Computational Chemistry</i> , 2003, , 1-41.	1.5	9
49	A dynamical definition of atomic clusters. <i>Journal of Chemical Physics</i> , 1991, 95, 3022-3023.	1.2	8
50	The melting transition of Ni <sub>7</sub> and Ni <sub>7</sub> H as modeled by a semi-empirical potential. <i>Chemical Physics Letters</i> , 1998, 295, 366-372.	1.2	7
51	Stationary tempering and the complex quadrature problem. <i>Journal of Chemical Physics</i> , 2002, 116, 3509-3520.	1.2	7
52	A comparison of energy estimators used in quantum Monte Carlo calculations. <i>Journal of Chemical Physics</i> , 1985, 83, 768-771.	1.2	5
53	On the encapsulation of nickel clusters by molecular nitrogen. <i>Journal of Chemical Physics</i> , 2004, 121, 475.	1.2	5
54	A numerical study of the asymptotic convergence characteristics of partial averaged and reweighted Fourier path integral methods. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2916-2925.	1.0	5

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55	Elephant's Toothpaste Used as a Qualitative Demonstration of Rate versus Temperature. Journal of Chemical Education, 2020, 97, 1061-1067.	1.1	4
56	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
57	Convergence characteristics of the cumulant expansion for Fourier path integrals. Physical Review E, 2010, 81, 066707.	0.8	3
58	Self-adaptive quadrature and numerical path integration. Journal of Chemical Physics, 2000, 113, 2522-2529.	1.2	2
59	Equilibrium and Dynamical Path Integral Methods. , 1999, , 213-245.		1
60	A numerical solution to the integral equation for atomic pair energies. Molecular Physics, 1978, 36, 655-667.	0.8	0
61	MONTE CARLO METHODS IN CHEMISTRY: A TUTORIAL. , 1998, , 529-579.		0
62	Monte Carlo Method for Real-Time Path Integration. AIP Conference Proceedings, 2003, , .	0.3	0
63	A(nother) Modification of the Ammonia Fountain Demonstration. Journal of Chemical Education, 2017, 94, 1397-1398.	1.1	0
64	Numerical Investigation of the Cumulant Expansion for Fourier Path Integrals. Lecture Notes in Computer Science, 2012, , 13-22.	1.0	0