Jimme Doll

List of Publications by Year
in descending order

29 papers	1,934 citations	430843 18 h-index	526264 27 g-index
29 all docs	29 docs citations	29 times ranked	955 citing authors

#	Article	IF	Citations
1	Brownian dynamics as smart Monte Carlo simulation. Journal of Chemical Physics, 1978, 69, 4628-4633.	3.0	387
2	Reducing quasiâ€ergodic behavior in Monte Carlo simulations by Jâ€walking: Applications to atomic clusters. Journal of Chemical Physics, 1990, 93, 2769-2784.	3.0	291
3	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.	3.0	240
4	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.	3.0	183
5	Equilibrium and Dynamical Fourier Path Integral Methods. Advances in Chemical Physics, 2007, , 61-127.	0.3	165
6	A variational Monte Carlo study of argon, neon, and helium clusters. Journal of Chemical Physics, 1991, 95, 3506-3520.	3.0	71
7	ExtendingJwalking to quantum systems: Applications to atomic clusters. Journal of Chemical Physics, 1992, 97, 5713-5731.	3.0	70
8	COMPUTATIONAL STUDIES OF CLUSTERS:Methods and Results. Annual Review of Physical Chemistry, 1996, 47, 43-80.	10.8	70
9	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.	3.0	66
10	The quantum dynamics of hydrogen and deuterium on the Pd(111) surface: A path integral transition state theory study. Journal of Chemical Physics, 1993, 99, 8183-8193.	3.0	59
11	An infinite swapping approach to the rare-event sampling problem. Journal of Chemical Physics, 2011, 135, 134111.	3.0	47
12	On the Infinite Swapping Limit for Parallel Tempering. Multiscale Modeling and Simulation, 2012, 10, 986-1022.	1.6	42
13	A heat capacity estimator for Fourier path integral simulations. Journal of Chemical Physics, 2000, 112, 3990-3996.	3.0	41
14	Optimal series representations for numerical path integral simulations. Journal of Chemical Physics, 2002, 117, 7448-7463.	3.0	41
15	Numerical implementation of some reweighted path integral methods. Journal of Chemical Physics, 2003, 119, 4641-4654.	3.0	25
16	Stationary Phase Monte Carlo Methods. Advances in Chemical Physics, 2007, , 289-304.	0.3	24
17	A j-walking algorithm for microcanonical simulations: Applications to Lennard-Jones clusters. Journal of Chemical Physics, 1998, 109, 1643-1647.	3.0	21
18	Overcoming the Rare Event Sampling Problem in Biological Systems with Infinite Swapping. Journal of Chemical Theory and Computation, 2013, 9, 4215-4224.	5.3	21

#	Article	IF	Citations
19	Rare-event sampling: Occupation-based performance measures for parallel tempering and infinite swapping Monte Carlo methods. Journal of Chemical Physics, 2012, 137, 204112.	3.0	19
20	Locating transition states using doubleâ€ended classical trajectories. Journal of Chemical Physics, 1994, 101, 10458-10463.	3.0	16
21	On performance measures for infinite swapping Monte Carlo methods. Journal of Chemical Physics, 2015, 142, 024111.	3.0	12
22	Fourier path integral Monte Carlo method for the calculation of the microcanonical density of states. Journal of Chemical Physics, 1994, 101, 848-849.	3.0	9
23	A Simple Method for Calculating Quantum Effects on the Temperature Dependence of Bimolecular Reaction Rates:Â Application to H2+ H â†' H + H2and CH4+ H â†' CH3+ H2. Journal of the American Chemical Society, 2000, 122, 9189-9195.	13.7	6
24	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.	2.0	5
25	Short Review of Recent Developments for Path Integral Techniques. AIP Conference Proceedings, 2003, , .	0.4	1
26	Spatial Averaging: Sampling Enhancement for Exploring Configurational Space of Atomic Clusters and Biomolecules. Journal of Chemical Theory and Computation, 2014, 10, 4284-4296.	5.3	1
27	Thermodynamic integration methods, infinite swapping, and the calculation of generalized averages. Journal of Chemical Physics, 2017, 146, 134111.	3.0	1
28	MONTE CARLO METHODS IN CHEMISTRY: A TUTORIAL. , 1998, , 529-579.		0
29	Monte Carlo Method for Real-Time Path Integration. AIP Conference Proceedings, 2003, , .	0.4	0