Michael F Herman

List of Publications by Year
in descending order

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56 papers	2,180 citations	394421 19 h-index	233421 45 g-index
57 all docs	57 docs citations	57 times ranked	900 citing authors

#	Article	IF	Citations
1	Surface hopping, transition state theory and decoherence. I. Scattering theory and time-reversibility. Journal of Chemical Physics, 2015, 143, 134106.	3.0	20
2	Time dependent semiclassical tunneling through one dimensional barriers using only real valued trajectories. Journal of Chemical Physics, 2015, 143, 164110.	3.0	0
3	Improving the Efficiency of Monte Carlo Surface Hopping Calculations. Journal of Physical Chemistry B, 2014, 118, 8026-8033.	2.6	4
4	Analysis of a surface hopping expansion that includes hops in classically forbidden regions. Chemical Physics, 2014, 433, 12-21.	1.9	4
5	A justification for the use of approximate transition amplitudes in semiclassical surface hopping. Molecular Physics, 2011, 109, 1581-1592.	1.7	3
6	The calculation of multidimensional semiclassical wave functions in the forbidden region using real valued coordinates. Journal of Chemical Physics, 2010, 133, 114108.	3.0	3
7	A singularity free surface hopping expansion for the multistate wave function. Journal of Chemical Physics, 2009, 131, 214108.	3.0	1
8	Semiclassical Nonadiabatic Surface-hopping Wave Function Expansion at Low Energies: Hops in the Forbidden Region. Journal of Physical Chemistry B, 2008, 112, 15966-15972.	2.6	5
9	An analysis through order â„2 of a surface hopping expansion of the nonadiabatic wave function. Journal of Chemical Physics, 2008, 128, 114105.	3.0	13
10	Using an r-dependent Gaussian width in calculations of the globally uniform semiclassical wave function. Journal of Chemical Physics, 2007, 126, 034104.	3.0	2
11	On the Importance of the Classically Forbidden Region in Calculations of the Relaxation Rate for High-Frequency Vibrations:â€‰ A Model Calculation. Journal of Physical Chemistry A, 2007, 111, 10186-10190.	2.5	0
12	Nonadiabatic Scattering Problems in Liquid-State Vibrational Relaxation. Advances in Chemical Physics, 2007, , 577-602.	0.3	1
13	Analysis and Evaluation of Ionization Potentials, Electron Affinities, and Excitation Energies by the Equations of Motion-Green's Function Method. Advances in Chemical Physics, 2007, , 1-69.	0.3	185
14	Numerical study of the accuracy and efficiency of various approaches for Monte Carlo surface hopping calculations. Journal of Chemical Physics, 2005, 122, 094104.	3.0	20
15	Toward an Accurate and Efficient Semiclassical Surface Hopping Procedure for Nonadiabatic Problems. Journal of Physical Chemistry A, 2005, 109, 9196-9205.	2.5	17
16	Globally uniform semiclassical surface-hopping wave function for nonadiabatic scattering. Journal of Chemical Physics, 2004, 120, 7383-7390.	3.0	12
17	Phase corrected higher-order expression for surface hopping transition amplitudes in nonadiabatic scattering problems. Journal of Chemical Physics, 2003, 119, 11048-11057.	3.0	13
18	Semiclassical Surface Hopping HâˆK Propagator: Application to Two-Dimensional, Two-Surface Problemsâ€. Journal of Physical Chemistry B, 2001, 105, 6562-6569.	2.6	25

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19	A Length Scale Dependent Model for Stress Relaxation in Polymer Melts. Macromolecules, 2001, 34, 4580-4590.	4.8	3
20	Recent nuclear magnetic resonance experiments on polymer melts: Comments. Journal of Chemical Physics, 2000, 112, 3040-3044.	3.0	6
21	Using Force Field Simulations for the Evaluation of the Monomer Parameters for the Calculation of Diffusion Constants for Long Chain Polymer Melts. Macromolecules, 2000, 33, 3932-3939.	4.8	4
22	Choosing a good representation of the quantum state wave functions for semiclassical surface hopping calculations. Journal of Chemical Physics, 1999, 111, 10427-10435.	3.0	23
23	Optimal representation for semiclassical surface hopping methods. Journal of Chemical Physics, 1999, 110, 4141-4151.	3.0	30
24	Improved treatment of the lateral-reptative mixing and approximate analytical expressions for the lateral motion model of polymer melts. Journal of Chemical Physics, 1999, 110, 8792-8801.	3.0	6
25	The development of semiclassical dynamical methods and their application to vibrational relaxation in condensed-phase systems. International Journal of Quantum Chemistry, 1998, 70, 897-907.	2.0	9
26	A quantitative theory of linear chain polymer dynamics in the melt. IV. Comparison with experimental diffusion constant data. Journal of Chemical Physics, 1998, 108, 5122-5129.	3.0	6
27	Model calculations of resonant vibration to vibration transition probabilities in clusters. Journal of Chemical Physics, 1998, 109, 4726-4733.	3.0	4
28	Comparison of theoretical methods for resonant vibrationâ€“vibration energy transfer in liquids. Journal of Chemical Physics, 1998, 108, 2903-2911.	3.0	8
29	An Explanation for the Experimental Data on the Motion of Rings and Linear Chains in Melts and Microgels. Macromolecules, 1996, 29, 6349-6350.	4.8	3
30	A quantitative theory of linear chain polymer dynamics in the melt. I. General scaling behavior. Journal of Chemical Physics, 1996, 105, 1153-1161.	3.0	14
31	A quantitative theory of linear chain polymer dynamics in the melt. II. Comparison with simulation data. Journal of Chemical Physics, 1996, 105, 1162-1174.	3.0	9
32	A quantitative theory of linear chain polymer dynamics in the melt. III. Dependence of quantities on bead location along the chain contour. Journal of Chemical Physics, 1996, 105, 2463-2470.	3.0	4
33	Enzymatic polymerizations using surfactant microstructures and the preparation of polymer-ferrite composites. Applied Biochemistry and Biotechnology, 1995, 51-52, 241-252.	2.9	12
34	Viscoelastic response of bidisperse melts in the lateral motion model. Journal of Chemical Physics, 1995, 102, 7700-7707.	3.0	7
35	Determining nuclear hyperfine populations in the ground electronic state of atomic hydrogen produced by the 193 nm photolysis of HBr. Journal of Chemical Physics, 1995, 103, 5864-5867.	3.0	6
36	The role of correlated many chain motions in linear chain polymer melts. Journal of Chemical Physics, 1995, 103, 4324-4332.	3.0	16

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37	A semiclassical surface hopping propagator for nonadiabatic problems. Journal of Chemical Physics, 1995, 103, 8081-8097.	3.0	72
38	Semiclassical surfaceâ€hopping approximations for the calculation of solventâ€induced vibrationalâ€relaxation rate constants. Journal of Chemical Physics, 1994, 101, 7520-7527.	3.0	26
39	Analysis of the statistical errors in conditioned real time path integral methods. Journal of Chemical Physics, 1993, 99, 5087-5090.	3.0	10
40	An approximate discretized real time path integral simulation method for nearly classical systems. Journal of Chemical Physics, 1993, 98, 6975-6981.	3.0	5
41	Realâ€time pathâ€integral simulation of vibrational transition probabilities of small molecules in clusters: Theory and application to Br2in Ar. Journal of Chemical Physics, 1992, 96, 5999-6009.	3.0	13
42	A nonreptation model for polymer dynamics in the melt and concentrated solutions. Journal of Chemical Physics, 1990, 92, 2043-2054.	3.0	20
43	A NON-MARKOVIAN MODEL FOR PARTICLE MOTION IN FLUIDIZED BEDS. Chemical Engineering Communications, 1987, 56, 203-209.	2.6	0
44	Solvent induced vibrational relaxation in diatomics. I. Derivation of a local relaxation rate. Journal of Chemical Physics, 1987, 87, 4779-4793.	3.0	32
45	Solvent induced vibrational population relaxation in diatomics. II. Simulation for Br2in Ar. Journal of Chemical Physics, 1987, 87, 4794-4801.	3.0	22
46	Comparison of the propagation of semiclassical frozen Gaussian wave functions with quantum propagation for a highly excited anharmonic oscillator. Journal of Chemical Physics, 1986, 84, 326-334.	3.0	271
47	Time reversal and unitarity in the frozen Gaussian approximation for semiclassical scattering. Journal of Chemical Physics, 1986, 85, 2069-2076.	3.0	76
48	Nonadiabatic semiclassical scattering. III. Time dependent surface hopping formalism. Journal of Chemical Physics, 1985, 82, 3666-3673.	3.0	34
49	Numerical comparison of generalized surface hopping, classical analog, and selfâ€consistent eikonal approximations for nonadiabatic scattering. Journal of Chemical Physics, 1985, 82, 4509-4516.	3.0	19
50	Analysis of the relative phases of contributions to the primitive semiclassicalSmatrix. Molecular Physics, 1985, 56, 525-539.	1.7	3
51	Nonadiabatic semiclassical scattering. II. Solution of twoâ€dimensional models and comparison with quantum results. Journal of Chemical Physics, 1984, 81, 764-774.	3.0	42
52	Nonadiabatic semiclassical scattering. I. Analysis of generalized surface hopping procedures. Journal of Chemical Physics, 1984, 81, 754-763.	3.0	172
53	A semiclasical justification for the use of non-spreading wavepackets in dynamics calculations. Chemical Physics, 1984, 91, 27-34.	1.9	687
54	Monte Carlo simulation of solvent effects on vibrational and electronic spectra. Journal of Chemical Physics, 1983, 78, 4103-4117.	3.0	69

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55	A new uniform semiclassical wave function for single surface and multisurface scattering. Journal of Chemical Physics, 1983, 79, 2771-2778.	3.0	17
56	Generalization of the geometric optical series approach for nonadiabatic scattering problems. Journal of Chemical Physics, 1982, 76, 2949-2958.	3.0	89