Michael F Herman

List of Publications by Year
in descending order

56 papers	2,180 citations	393982 19 h-index	233125 45 g-index
57 all docs	57 docs citations	57 times ranked	900 citing authors

#	Article	IF	Citations
1	A semiclasical justification for the use of non-spreading wavepackets in dynamics calculations. Chemical Physics, 1984, 91, 27-34.	0.9	687
2	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.	1.2	271
3	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
4	Nonadiabatic semiclassical scattering. I. Analysis of generalized surface hopping procedures. Journal of Chemical Physics, 1984, 81, 754-763.	1.2	172
5	Generalization of the geometric optical series approach for nonadiabatic scattering problems. Journal of Chemical Physics, 1982, 76, 2949-2958.	1.2	89
6	Time reversal and unitarity in the frozen Gaussian approximation for semiclassical scattering. Journal of Chemical Physics, 1986, 85, 2069-2076.	1.2	76
7	A semiclassical surface hopping propagator for nonadiabatic problems. Journal of Chemical Physics, 1995, 103, 8081-8097.	1.2	72
8	Monte Carlo simulation of solvent effects on vibrational and electronic spectra. Journal of Chemical Physics, 1983, 78, 4103-4117.	1.2	69
9	Nonadiabatic semiclassical scattering. II. Solution of twoâ€dimensional models and comparison with quantum results. Journal of Chemical Physics, 1984, 81, 764-774.	1.2	42
10	Nonadiabatic semiclassical scattering. III. Time dependent surface hopping formalism. Journal of Chemical Physics, 1985, 82, 3666-3673.	1.2	34
11	Solvent induced vibrational relaxation in diatomics. I. Derivation of a local relaxation rate. Journal of Chemical Physics, 1987, 87, 4779-4793.	1.2	32
12	Optimal representation for semiclassical surface hopping methods. Journal of Chemical Physics, 1999, 110, 4141-4151.	1.2	30
13	Semiclassical surfaceâ€hopping approximations for the calculation of solventâ€induced vibrationalâ€relaxation rate constants. Journal of Chemical Physics, 1994, 101, 7520-7527.	1.2	26
14	Semiclassical Surface Hopping Hâ^'K Propagator: Application to Two-Dimensional, Two-Surface Problemsâ€. Journal of Physical Chemistry B, 2001, 105, 6562-6569.	1.2	25
15	Choosing a good representation of the quantum state wave functions for semiclassical surface hopping calculations. Journal of Chemical Physics, 1999, 111, 10427-10435.	1.2	23
16	Solvent induced vibrational population relaxation in diatomics. II. Simulation for Br2in Ar. Journal of Chemical Physics, 1987, 87, 4794-4801.	1.2	22
17	A nonreptation model for polymer dynamics in the melt and concentrated solutions. Journal of Chemical Physics, 1990, 92, 2043-2054.	1.2	20
18	Numerical study of the accuracy and efficiency of various approaches for Monte Carlo surface hopping calculations. Journal of Chemical Physics, 2005, 122, 094104.	1.2	20

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19	Surface hopping, transition state theory and decoherence. I. Scattering theory and time-reversibility. Journal of Chemical Physics, 2015, 143, 134106.	1.2	20
20	Numerical comparison of generalized surface hopping, classical analog, and selfâ€consistent eikonal approximations for nonadiabatic scattering. Journal of Chemical Physics, 1985, 82, 4509-4516.	1.2	19
21	A new uniform semiclassical wave function for single surface and multisurface scattering. Journal of Chemical Physics, 1983, 79, 2771-2778.	1.2	17
22	Toward an Accurate and Efficient Semiclassical Surface Hopping Procedure for Nonadiabatic Problems. Journal of Physical Chemistry A, 2005, 109, 9196-9205.	1.1	17
23	The role of correlated many chain motions in linear chain polymer melts. Journal of Chemical Physics, 1995, 103, 4324-4332.	1.2	16
24	A quantitative theory of linear chain polymer dynamics in the melt. I. General scaling behavior. Journal of Chemical Physics, 1996, 105, 1153-1161.	1.2	14
25	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.	1.2	13
26	Phase corrected higher-order expression for surface hopping transition amplitudes in nonadiabatic scattering problems. Journal of Chemical Physics, 2003, 119, 11048-11057.	1.2	13
27	An analysis through order â„2 of a surface hopping expansion of the nonadiabatic wave function. Journal of Chemical Physics, 2008, 128, 114105.	1.2	13
28	Enzymatic polymerizations using surfactant microstructures and the preparation of polymer-ferrite composites. Applied Biochemistry and Biotechnology, 1995, 51-52, 241-252.	1.4	12
29	Globally uniform semiclassical surface-hopping wave function for nonadiabatic scattering. Journal of Chemical Physics, 2004, 120, 7383-7390.	1.2	12
30	Analysis of the statistical errors in conditioned real time path integral methods. Journal of Chemical Physics, 1993, 99, 5087-5090.	1.2	10
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.	1.2	9
32	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.	1.0	9
33	Comparison of theoretical methods for resonant vibrationâ€“vibration energy transfer in liquids. Journal of Chemical Physics, 1998, 108, 2903-2911.	1.2	8
34	Viscoelastic response of bidisperse melts in the lateral motion model. Journal of Chemical Physics, 1995, 102, 7700-7707.	1.2	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.	1.2	6
36	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.	1.2	6

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37	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.	1.2	6
38	Recent nuclear magnetic resonance experiments on polymer melts: Comments. Journal of Chemical Physics, 2000, 112, 3040-3044.	1.2	6
39	An approximate discretized real time path integral simulation method for nearly classical systems. Journal of Chemical Physics, 1993, 98, 6975-6981.	1.2	5
40	Semiclassical Nonadiabatic Surface-hopping Wave Function Expansion at Low Energies: Hops in the Forbidden Region. Journal of Physical Chemistry B, 2008, 112, 15966-15972.	1.2	5
41	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.	1.2	4
42	Model calculations of resonant vibration to vibration transition probabilities in clusters. Journal of Chemical Physics, 1998, 109, 4726-4733.	1.2	4
43	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.	2.2	4
44	Improving the Efficiency of Monte Carlo Surface Hopping Calculations. Journal of Physical Chemistry B, 2014, 118, 8026-8033.	1.2	4
45	Analysis of a surface hopping expansion that includes hops in classically forbidden regions. Chemical Physics, 2014, 433, 12-21.	0.9	4
46	Analysis of the relative phases of contributions to the primitive semiclassicalSmatrix. Molecular Physics, 1985, 56, 525-539.	0.8	3
47	An Explanation for the Experimental Data on the Motion of Rings and Linear Chains in Melts and Microgels. Macromolecules, 1996, 29, 6349-6350.	2.2	3
48	A Length Scale Dependent Model for Stress Relaxation in Polymer Melts. Macromolecules, 2001, 34, 4580-4590.	2.2	3
49	The calculation of multidimensional semiclassical wave functions in the forbidden region using real valued coordinates. Journal of Chemical Physics, 2010, 133, 114108.	1.2	3
50	A justification for the use of approximate transition amplitudes in semiclassical surface hopping. Molecular Physics, 2011, 109, 1581-1592.	0.8	3
51	Using an r-dependent Gaussian width in calculations of the globally uniform semiclassical wave function. Journal of Chemical Physics, 2007, 126, 034104.	1.2	2
52	Nonadiabatic Scattering Problems in Liquid-State Vibrational Relaxation. Advances in Chemical Physics, 2007, , 577-602.	0.3	1
53	A singularity free surface hopping expansion for the multistate wave function. Journal of Chemical Physics, 2009, 131, 214108.	1.2	1
54	A NON-MARKOVIAN MODEL FOR PARTICLE MOTION IN FLUIDIZED BEDS. Chemical Engineering Communications, 1987, 56, 203-209.	1.5	0

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55	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.	1.1	0
56	Time dependent semiclassical tunneling through one dimensional barriers using only real valued trajectories. Journal of Chemical Physics, 2015, 143, 164110.	1.2	0