Michael F Herman

List of Publications by Year in Descending Order

56 papers	2,029 citations	19 h-index	44 g-index
57 ext. papers	2,088 ext. citations	3.6 avg, IF	4.7 L-index

#	Paper	IF	Citations
56	Surface hopping, transition state theory and decoherence. I. Scattering theory and time-reversibility. *Journal of Chemical Physics*, **2015**, 143, 134106	3.9	18
55	Time dependent semiclassical tunneling through one dimensional barriers using only real valued trajectories. *Journal of Chemical Physics*, **2015**, 143, 164110	3.9	
54	Improving the efficiency of Monte Carlo surface hopping calculations. *Journal of Physical Chemistry B*, **2014**, 118, 8026-33	3.4	4
53	Analysis of a surface hopping expansion that includes hops in classically forbidden regions. *Chemical Physics*, **2014**, 433, 12-21	2.3	4
52	A justification for the use of approximate transition amplitudes in semiclassical surface hopping. *Molecular Physics*, **2011**, 109, 1581-1592	1.7	3
51	The calculation of multidimensional semiclassical wave functions in the forbidden region using real valued coordinates. *Journal of Chemical Physics*, **2010**, 133, 114108	3.9	2
50	A singularity free surface hopping expansion for the multistate wave function. *Journal of Chemical Physics*, **2009**, 131, 214108	3.9	1
49	Semiclassical nonadiabatic surface-hopping wave function expansion at low energies: hops in the forbidden region. *Journal of Physical Chemistry B*, **2008**, 112, 15966-72	3.4	5
48	An analysis through order variant Planckžs constant over 2pi(2) of a surface hopping expansion of the nonadiabatic wave function. *Journal of Chemical Physics*, **2008**, 128, 114105	3.9	13
47	On the importance of the classically forbidden region in calculations of the relaxation rate for high-frequency vibrations: a model calculation. *Journal of Physical Chemistry A*, **2007**, 111, 10186-90	2.8	
46	Nonadiabatic Scattering Problems in Liquid-State Vibrational Relaxation. *Advances in Chemical Physics*, **2007**, 577-602		1
45	Analysis and Evaluation of Ionization Potentials, Electron Affinities, and Excitation Energies by the Equations of Motion□Greenžs Function Method. *Advances in Chemical Physics*, **2007**, 1-69		169
44	Using an r-dependent Gaussian width in calculations of the globally uniform semiclassical wave function. *Journal of Chemical Physics*, **2007**, 126, 034104	3.9	2
43	Toward an accurate and efficient semiclassical surface hopping procedure for nonadiabatic problems. *Journal of Physical Chemistry A*, **2005**, 109, 9196-205	2.8	17
42	Numerical study of the accuracy and efficiency of various approaches for Monte Carlo surface hopping calculations. *Journal of Chemical Physics*, **2005**, 122, 094104	3.9	20
41	Globally uniform semiclassical surface-hopping wave function for nonadiabatic scattering. *Journal of Chemical Physics*, **2004**, 120, 7383-90	3.9	12
40	Phase corrected higher-order expression for surface hopping transition amplitudes in nonadiabatic scattering problems. *Journal of Chemical Physics*, **2003**, 119, 11048-11057	3.9	13

39	Semiclassical Surface Hopping HK Propagator: Application to Two-Dimensional, Two-Surface Problems *Journal of Physical Chemistry B*, **2001**, 105, 6562-6569	3.4	25
38	A Length Scale Dependent Model for Stress Relaxation in Polymer Melts. *Macromolecules*, **2001**, 34, 4580-4590	3.5	3
37	Recent nuclear magnetic resonance experiments on polymer melts: Comments. *Journal of Chemical Physics*, **2000**, 112, 3040-3044	3.9	5
36	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	5.5	4
35	Choosing a good representation of the quantum state wave functions for semiclassical surface hopping calculations. *Journal of Chemical Physics*, **1999**, 111, 10427-10435	3.9	23
34	Optimal representation for semiclassical surface hopping methods. *Journal of Chemical Physics*, **1999**, 110, 4141-4151	3.9	29
33	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	3.9	6
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	2.1	9
31	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	3.9	6
30	Model calculations of resonant vibration to vibration transition probabilities in clusters. *Journal of Chemical Physics*, **1998**, 109, 4726-4733	3.9	4
29	Comparison of theoretical methods for resonant vibration ibration energy transfer in liquids. *Journal of Chemical Physics*, **1998**, 108, 2903-2911	3.9	7
28	An Explanation for the Experimental Data on the Motion of Rings and Linear Chains in Melts and Microgels. *Macromolecules*, **1996**, 29, 6349-6350	5.5	3
27	A quantitative theory of linear chain polymer dynamics in the melt. I. General scaling behavior. *Journal of Chemical Physics*, **1996**, 105, 1153-1161	3.9	12
26	A quantitative theory of linear chain polymer dynamics in the melt. II. Comparison with simulation data. *Journal of Chemical Physics*, **1996**, 105, 1162-1174	3.9	8
25	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	3.9	4
24	Enzymatic polymerizations using surfactant microstructures and the preparation of polymer-ferrite composites. *Applied Biochemistry and Biotechnology*, **1995**, 51-52, 241-252	3.2	10
23	Viscoelastic response of bidisperse melts in the lateral motion model. *Journal of Chemical Physics*, **1995**, 102, 7700-7707	3.9	7
22	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	3.9	6

21	The role of correlated many chain motions in linear chain polymer melts. *Journal of Chemical Physics*, **1995**, 103, 4324-4332	3.9	16
20	A semiclassical surface hopping propagator for nonadiabatic problems. *Journal of Chemical Physics*, **1995**, 103, 8081-8097	3.9	69
19	Semiclassical surface-hopping approximations for the calculation of solvent-induced vibrational-relaxation rate constants. *Journal of Chemical Physics*, **1994**, 101, 7520-7527	3.9	25
18	Analysis of the statistical errors in conditioned real time path integral methods. *Journal of Chemical Physics*, **1993**, 99, 5087-5090	3.9	9
17	An approximate discretized real time path integral simulation method for nearly classical systems. *Journal of Chemical Physics*, **1993**, 98, 6975-6981	3.9	5
16	Real-time path-integral simulation of vibrational transition probabilities of small molecules in clusters: Theory and application to Br2 in Ar. *Journal of Chemical Physics*, **1992**, 96, 5999-6009	3.9	12
15	A nonreptation model for polymer dynamics in the melt and concentrated solutions. *Journal of Chemical Physics*, **1990**, 92, 2043-2054	3.9	19
14	A NON-MARKOVIAN MODEL FOR PARTICLE MOTION IN FLUIDIZED BEDS. *Chemical Engineering Communications*, **1987**, 56, 203-209	2.2	
13	Solvent induced vibrational relaxation in diatomics. I. Derivation of a local relaxation rate. *Journal of Chemical Physics*, **1987**, 87, 4779-4793	3.9	31
12	Solvent induced vibrational population relaxation in diatomics. II. Simulation for Br2 in Ar. *Journal of Chemical Physics*, **1987**, 87, 4794-4801	3.9	19
11	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	3.9	256
10	Time reversal and unitarity in the frozen Gaussian approximation for semiclassical scattering. *Journal of Chemical Physics*, **1986**, 85, 2069-2076	3.9	72
9	Nonadiabatic semiclassical scattering. III. Time dependent surface hopping formalism. *Journal of Chemical Physics*, **1985**, 82, 3666-3673	3.9	34
8	Numerical comparison of generalized surface hopping, classical analog, and self-consistent eikonal approximations for nonadiabatic scattering. *Journal of Chemical Physics*, **1985**, 82, 4509-4516	3.9	19
7	Analysis of the relative phases of contributions to the primitive semiclassical S matrix. *Molecular Physics*, **1985**, 56, 525-539	1.7	3
6	Nonadiabatic semiclassical scattering. II. Solution of two-dimensional models and comparison with quantum results. *Journal of Chemical Physics*, **1984**, 81, 764-774	3.9	38
5	Nonadiabatic semiclassical scattering. I. Analysis of generalized surface hopping procedures. *Journal of Chemical Physics*, **1984**, 81, 754-763	3.9	151
4	A semiclasical justification for the use of non-spreading wavepackets in dynamics calculations. *Chemical Physics*, **1984**, 91, 27-34	2.3	625

3	Monte Carlo simulation of solvent effects on vibrational and electronic spectra. *Journal of Chemical Physics*, **1983**, 78, 4103-4117	3.9	65
2	A new uniform semiclassical wave function for single surface and multisurface scattering. *Journal of Chemical Physics*, **1983**, 79, 2771-2778	3.9	17
1	Generalization of the geometric optical series approach for nonadiabatic scattering problems. *Journal of Chemical Physics*, **1982**, 76, 2949-2958	3.9	86