Sherwin J Singer

List of Publications by Year
in descending order

87 papers	4,941 citations	101543 36 h-index	91884 69 g-index
89 all docs	89 docs citations	89 times ranked	3958 citing authors

#	Article	IF	Citations
1	Role of Water in Electron-Initiated Processes and Radical Chemistry:â€‰ Issues and Scientific Advances. Chemical Reviews, 2005, 105, 355-390.	47.7	560
2	Density functional theory of nonuniform polyatomic systems. I. General formulation. Journal of Chemical Physics, 1986, 85, 5971-5976.	3.0	358
3	Free energy functions in the extended RISM approximation. Molecular Physics, 1985, 55, 621-625.	1.7	331
4	Hydration Dynamics and Time Scales of Coupled Waterâˆ’Protein Fluctuations. Journal of the American Chemical Society, 2007, 129, 3376-3382.	13.7	232
5	Density functional theory of nonuniform polyatomic systems. II. Rational closures for integral equations. Journal of Chemical Physics, 1986, 85, 5977-5982.	3.0	223
6	Potential models for simulations of the solvated proton in water. Journal of Chemical Physics, 1998, 109, 5547-5564.	3.0	187
7	Graph Theoretical Generation and Analysis of Hydrogen-Bonded Structures with Applications to the Neutral and Protonated Water Cube and Dodecahedral Clusters. Journal of Physical Chemistry A, 1998, 102, 2824-2832.	2.5	182
8	Theory of diatomic molecule photodissociation: Electronic angular momentum influence on fragment and fluorescence cross sections. Journal of Chemical Physics, 1983, 79, 6060-6085.	3.0	135
9	Computational Analysis of the Potential Energy Surfaces of Glycerol in the Gas and Aqueous Phases:Â Effects of Level of Theory, Basis Set, and Solvation on Strongly Intramolecularly Hydrogen-Bonded Systems. Journal of the American Chemical Society, 2001, 123, 11743-11754.	13.7	133
10	Model for the Waterâˆ’Amorphous Silica Interface:â€‰ The Undissociated Surface. Journal of Physical Chemistry B, 2007, 111, 11181-11193.	2.6	125
11	On the use of graph invariants for efficiently generating hydrogen bond topologies and predicting physical properties of water clusters and ice. Journal of Chemical Physics, 2001, 114, 2527-2540.	3.0	110
12	Potential energy surfaces and vibrational spectra of H5O2+ and larger hydrated proton complexes. International Journal of Quantum Chemistry, 1995, 56, 657-668.	2.0	89
13	Hydrogen-Bond Topology and the IceVII/VIIIand Icelh/XIProton-Ordering Phase Transitions. Physical Review Letters, 2005, 94, 135701.	7.8	86
14	Short H-bonds and spontaneous self-dissociation in (H2O)20: Effects of H-bond topology. Journal of Chemical Physics, 2003, 118, 3583-3588.	3.0	83
15	DNA Binding to the Silica Surface. Journal of Physical Chemistry B, 2015, 119, 11030-11040.	2.6	82
16	Stochastic molecular dynamics study of cyclohexane isomerization. The Journal of Physical Chemistry, 1988, 92, 3261-3267.	2.9	74
17	A density functional treatment of the hard dumbbell freezing transition. Journal of Chemical Physics, 1987, 87, 4853-4858.	3.0	73
18	Stripe Melting in a Two-Dimensional System with Competing Interactions. Physical Review Letters, 2000, 84, 4657-4660.	7.8	71

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19	Enumeration and Evaluation of the Water Hexamer Cage Structure. Journal of Physical Chemistry A, 2000, 104, 752-757.	2.5	61
20	The waterâ€“amorphous silica interface: Analysis of the Stern layer and surface conduction. Journal of Chemical Physics, 2011, 134, 024705.	3.0	60
21	Hydrogen bond topology and the ice VII/VIII and Ih/XI proton ordering phase transitions. Physical Review E, 2006, 73, 056113.	2.1	59
22	Monte Carlo study of fluidâ€“plastic crystal coexistence in hard dumbbells. Journal of Chemical Physics, 1990, 93, 1278-1286.	3.0	54
23	Origin of Slow Relaxation Following Photoexcitation of W7 in Myoglobin and the Dynamics of Its Hydration Layer. Journal of Physical Chemistry B, 2008, 112, 16121-16134.	2.6	54
24	Photodissociation of Diatomic Molecules to Open Shell Atoms. Advances in Chemical Physics, 2007, , 1-113.	0.3	53
25	Structure and vibrational spectra of H[sup +](H[sub 2]O)[sub 8]: Is the excess proton in a symmetrical hydrogen bond?. Journal of Chemical Physics, 2000, 113, 5321.	3.0	47
26	Electro-osmotic flow of a model electrolyte. Physical Review E, 2005, 71, 041501.	2.1	47
27	A Molecular Dynamics Study of Lys-Trp-Lys:Â Structure and Dynamics in Solution Following Photoexcitation. Journal of Physical Chemistry B, 2006, 110, 10497-10508.	2.6	46
28	Electronic energy shifts of a sodium atom in argon clusters by simulated annealing. Journal of Chemical Physics, 1990, 93, 7187-7200.	3.0	45
29	Full Dimensional Quantum Calculations of Vibrational Energies of H5O2+. Journal of Physical Chemistry A, 2003, 107, 7142-7151.	2.5	45
30	The Dissociated Amorphous Silica Surface: Model Development and Evaluation. Journal of Chemical Theory and Computation, 2010, 6, 3456-3471.	5.3	45
31	Domain-array melting in the dipolar lattice gas. Physical Review B, 1992, 46, 5783-5786.	3.2	44
32	Topology versus temperature: Thermal behavior of H+(H2O)8 and H+(H2O)16. Journal of Chemical Physics, 2000, 112, 710-716.	3.0	42
33	Prediction of a Phase Transition to a Hydrogen Bond Ordered Form of Ice VI. Journal of Physical Chemistry B, 2005, 109, 21040-21046.	2.6	41
34	Layer buckling in smectic-Aliquid crystals and two-dimensional stripe phases. Physical Review E, 1993, 48, 2796-2804.	2.1	40
35	Molecular Dynamics Study of the Electric Double Layer and Nonlinear Spectroscopy at the Amorphous Silicaâ€“Water Interface. Journal of Physical Chemistry B, 2019, 123, 6364-6384.	2.6	40
36	Graph invariants for periodic systems: Towards predicting physical properties from the hydrogen bond topology of ice. Physical Review E, 2003, 67, 016114.	2.1	37

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37	Cross sections and angular distributions for individual fragment fine structure levels produced in oneâ€•and twoâ€photon photodissociation of NaH. Journal of Chemical Physics, 1984, 81, 3091-3101.	3.0	36
38	Domain energies of the dipolar lattice gas. The Journal of Physical Chemistry, 1992, 96, 1938-1950.	2.9	36
39	Global orientational order in model polar clusters. Journal of Chemical Physics, 1994, 101, 7856-7867.	3.0	35
40	Invariant imbedding solution of driven (inhomogeneous) and homogeneous SchrÃ¶dinger equations. Journal of Chemical Physics, 1982, 77, 1942-1950.	3.0	34
41	Electric-field-induced layer buckling in chiral smectic-Aliquid crystals. Physical Review E, 1998, 57, 3059-3062.	2.1	34
42	Multichannel quantum theory for propagation of second order transition amplitudes. Journal of Chemical Physics, 1987, 87, 4762-4778.	3.0	33
43	A reexamination of the ice III/IX hydrogen bond ordering phase transition. Journal of Chemical Physics, 2006, 125, 064506.	3.0	33
44	An AIMD Study of the CPD Repair Mechanism in Water: Reaction Free Energy Surface and Mechanistic Implications. Journal of Physical Chemistry B, 2011, 115, 3848-3859.	2.6	32
45	Non-monotonic dependence of electronic relaxation rate on solvent viscosity. Chemical Physics Letters, 1983, 99, 225-231.	2.6	31
46	Dissociation of a diatomic molecule to atomic fine structure states: Electronically nonadiabatic effects upon resonant twoâ€photon dissociation. Journal of Chemical Physics, 1984, 81, 3064-3090.	3.0	31
47	Computer simulations of a two-dimensional system with competing interactions. Physical Review E, 2002, 65, 036706.	2.1	31
48	An AIMD Study of CPD Repair Mechanism in Water: Role of Solvent in Ring Splitting. Journal of Physical Chemistry B, 2011, 115, 3860-3871.	2.6	30
49	Experimental evidence for surface freezing in supercooled n-alkane nanodroplets. Physical Chemistry Chemical Physics, 2013, 15, 6783.	2.8	30
50	Hydrogen bond ordering in ice V and the transition to ice XIII. Journal of Chemical Physics, 2008, 129, 164513.	3.0	29
51	Orientation, alignment, and hyperfine effects on dissociation of diatomic molecules to open shell atoms. Journal of Chemical Physics, 1986, 84, 3762-3770.	3.0	25
52	Electronic spectra of NaAr4and NaAr6: Isomerization and melting. Journal of Chemical Physics, 1992, 96, 7977-7991.	3.0	25
53	Correlation Function Quantum Monte Carlo Study of the Excited Vibrational States of H5O2+Ââ€. Journal of Physical Chemistry A, 2004, 108, 8691-8702.	2.5	25
54	Analysis of the Subcritical Carbon Dioxideâˆ'Water Interface. Journal of Physical Chemistry A, 2011, 115, 6285-6296.	2.5	24

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55	Photodissociation of homonuclear diatomics: Fine structure cross sections for Na2(X1Î£g+) â†' Na(2S1/2) +		

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73	Site Disorder in Ice VII Arising from Hydrogen Bond Fluctuations. Journal of Physical Chemistry A, 2009, 113, 12433-12438.	2.5	9
74	Mechanism of surface freezing of alkanes. Journal of Chemical Physics, 2020, 153, 224501.	3.0	9
75	Accurate non-local electronâ€"argon pseudopotential for condensed phase simulation. Chemical Physics Letters, 1991, 184, 571-578.	2.6	8
76	Multiconfigurational electronic wave functions without a reference configuration: Analysis of a simulated annealing strategy. Journal of Chemical Physics, 1990, 93, 7201-7212.	3.0	7
77	Is aluminum-argon (AlAr12) icosahedral?. The Journal of Physical Chemistry, 1992, 96, 5325-5331.	2.9	7
78	On the determination of the crystal-vapor surface free energy, and why a Gaussian expression can be accurate for a system far from Gaussian. Journal of Chemical Physics, 2016, 145, 054710.	3.0	6
79	Nonadiabatic effects on the photodissociation of diatomic molecules to open-shell atoms. The Journal of Physical Chemistry, 1987, 91, 5402-5409.	2.9	5
80	Biomolecules at the amorphous silica/water interface: Binding and fluorescence anisotropy of peptides. Colloids and Surfaces B: Biointerfaces, 2017, 157, 83-92.	5.0	5
81	Structural studies of Bacillus subtilis glutamine synthetase. Archives of Biochemistry and Biophysics, 1977, 178, 644-651.	3.0	4
82	Multiparticle Monte Carlo moves: Algorithm for solids with free-energy determination. Computer Physics Communications, 1990, 59, 463-470.	7.5	4
83	Dielectric Behavior near a Spherical Ion. Journal of Physical Chemistry B, 2021, 125, 2360-2371.	2.6	2
84	Surface freezing of n-octane nanodroplets. , 2013, , .		1
85	Dielectric spectrum of a DNA oligomer. Physical Review E, 2018, 98, .	2.1	1
86	Full Dimensional Quantum Calculations of Vibrational Energies of H5O+2.. ChemInform, 2003, 34, no.	0.0	0
87	Monte Carlo simulation of methyl chloride monolayer on the surface of graphite. Surface Science, 2005, 579, 141-156.	1.9	0