Sherwin J Singer

List of Publications by Year
in descending order

87 papers	4,941 citations	101384 36 h-index	91712 69 g-index
89 all docs	89 docs citations	89 times ranked	3958 citing authors

#	Article	IF	Citations
1	Dielectric Behavior near a Spherical Ion. Journal of Physical Chemistry B, 2021, 125, 2360-2371.	1.2	2
2	A theoretical study of polymorphism in VQIVYK fibrils. Biophysical Journal, 2021, 120, 1396-1416.	0.2	10
3	Mechanism of surface freezing of alkanes. Journal of Chemical Physics, 2020, 153, 224501.	1.2	9
4	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.	1.2	40
5	Dielectric spectrum of a DNA oligomer. Physical Review E, 2018, 98, .	0.8	1
6	Biomolecules at the amorphous silica/water interface: Binding and fluorescence anisotropy of peptides. Colloids and Surfaces B: Biointerfaces, 2017, 157, 83-92.	2.5	5
7	Polarization charge: Theory and applications to aqueous interfaces. Journal of Chemical Physics, 2016, 144, 164702.	1.2	13
8	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.	1.2	6
9	DNA Binding to the Silica Surface. Journal of Physical Chemistry B, 2015, 119, 11030-11040.	1.2	82
10	Displacements, Mean-Squared Displacements, and Codisplacements for the Calculation of Nonequilibrium Properties. Journal of Physical Chemistry B, 2014, 118, 8170-8178.	1.2	21
11	Experimental evidence for surface freezing in supercooled n-alkane nanodroplets. Physical Chemistry Chemical Physics, 2013, 15, 6783.	1.3	30
12	Surface freezing of n-octane nanodroplets. , 2013, , .		1
13	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.	1.2	32
14	Analysis of the Subcritical Carbon Dioxideâ^'Water Interface. Journal of Physical Chemistry A, 2011, 115, 6285-6296.	1.1	24
15	An AIMD Study of CPD Repair Mechanism in Water: Role of Solvent in Ring Splitting. Journal of Physical Chemistry B, 2011, 115, 3860-3871.	1.2	30
16	The waterâ€“amorphous silica interface: Analysis of the Stern layer and surface conduction. Journal of Chemical Physics, 2011, 134, 024705.	1.2	60
17	The Dissociated Amorphous Silica Surface: Model Development and Evaluation. Journal of Chemical Theory and Computation, 2010, 6, 3456-3471.	2.3	45
18	Site Disorder in Ice VII Arising from Hydrogen Bond Fluctuations. Journal of Physical Chemistry A, 2009, 113, 12433-12438.	1.1	9

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19	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.	1.2	54
20	Hydrogen bond ordering in ice V and the transition to ice XIII. Journal of Chemical Physics, 2008, 129, 164513.	1.2	29
21	Photodissociation of Diatomic Molecules to Open Shell Atoms. Advances in Chemical Physics, 2007, , 1-113.	0.3	53
22	Model for the Waterâ^'Amorphous Silica Interface:â€‰ The Undissociated Surface. Journal of Physical Chemistry B, 2007, 111, 11181-11193.	1.2	125
23	Hydration Dynamics and Time Scales of Coupled Waterâ^'Protein Fluctuations. Journal of the American Chemical Society, 2007, 129, 3376-3382.	6.6	232
24	Static and dynamic properties of the water/amorphous silica interface: a model for the undissociated surface. Journal of Computer-Aided Materials Design, 2007, 14, 53-63.	0.7	18
25	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.	1.2	46
26	A reexamination of the ice III/IX hydrogen bond ordering phase transition. Journal of Chemical Physics, 2006, 125, 064506.	1.2	33
27	Hydrogen bond topology and the ice VII/VIII and Ih/XI proton ordering phase transitions. Physical Review E, 2006, 73, 056113.	0.8	59
28	Monte Carlo simulation of methyl chloride monolayer on the surface of graphite. Surface Science, 2005, 579, 141-156.	0.8	0
29	Hydrogen bonding in cubic(H2O)8andOHâ^™(H2O)7clusters. Physical Review A, 2005, 71, .	1.0	23
30	Hydrogen-Bond Topology and the IceVII/VIIIand IceIh/XIProton-Ordering Phase Transitions. Physical Review Letters, 2005, 94, 135701.	2.9	86
31	Prediction of a Phase Transition to a Hydrogen Bond Ordered Form of Ice VI. Journal of Physical Chemistry B, 2005, 109, 21040-21046.	1.2	41
32	Role of Water in Electron-Initiated Processes and Radical Chemistry:â€‰ Issues and Scientific Advances. Chemical Reviews, 2005, 105, 355-390.	23.0	560
33	Electro-osmotic flow of a model electrolyte. Physical Review E, 2005, 71, 041501.	0.8	47
34	Correlation Function Quantum Monte Carlo Study of the Excited Vibrational States of H5O2+Ââ€. Journal of Physical Chemistry A, 2004, 108, 8691-8702.	1.1	25
35	Full Dimensional Quantum Calculations of Vibrational Energies of H5O+2.. ChemInform, 2003, 34, no.	0.1	0
36	Graph invariants for periodic systems: Towards predicting physical properties from the hydrogen bond topology of ice. Physical Review E, 2003, 67, 016114.	0.8	37

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37	Short H-bonds and spontaneous self-dissociation in (H2O)20: Effects of H-bond topology. Journal of Chemical Physics, 2003, 118, 3583-3588.	1.2	83
38	Full Dimensional Quantum Calculations of Vibrational Energies of H5O2+. Journal of Physical Chemistry A, 2003, 107, 7142-7151.	1.1	45
39	Computer simulations of a two-dimensional system with competing interactions. Physical Review E, 2002, 65, 036706.	0.8	31
40	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.	6.6	133
41	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.	1.2	110
42	Scaling theory for two-dimensional systems with competing interactions. Physical Review E, 2001, 64, 016118.	0.8	16
43	Topology versus temperature: Thermal behavior of H+(H2O)8 and H+(H2O)16. Journal of Chemical Physics, 2000, 112, 710-716.	1.2	42
44	Buckling induced by dilative strain in two- and three-dimensional layered materials. Physical Review E, 2000, 62, 3736-3746.	0.8	13
45	Stripe Melting in a Two-Dimensional System with Competing Interactions. Physical Review Letters, 2000, 84, 4657-4660.	2.9	71
46	Enumeration and Evaluation of the Water Hexamer Cage Structure. Journal of Physical Chemistry A, 2000, 104, 752-757.	1.1	61
47	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.	1.2	47
48	Potential models for simulations of the solvated proton in water. Journal of Chemical Physics, 1998, 109, 5547-5564.	1.2	187
49	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.	1.1	182
50	Electric-field-induced layer buckling in chiral smectic-Aliquid crystals. Physical Review E, 1998, 57, 3059-3062.	0.8	34
51	Ion solvation in model polar clusters. Journal of Chemical Physics, 1996, 105, 3700-3714.	1.2	22
52	Potential energy surfaces and vibrational spectra of H5O2+ and larger hydrated proton complexes. International Journal of Quantum Chemistry, 1995, 56, 657-668.	1.0	89
53	Orientational ordering and anisotropy in model polar clusters. Journal of Chemical Physics, 1995, 103, 1913-1921.	1.2	21
54	Local-mode analysis of complex zeolite vibrations: sodalite. The Journal of Physical Chemistry, 1994, 98, 12670-12678.	2.9	11

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55	Local-mode analysis of complex zeolite vibrations: Zeolite-A. The Journal of Physical Chemistry, 1994, 98, 12679-12686.	2.9	18
56	Global orientational order in model polar clusters. Journal of Chemical Physics, 1994, 101, 7856-7867.	1.2	35
57	Layer buckling in smectic-Aliquid crystals and two-dimensional stripe phases. Physical Review E, 1993, 48, 2796-2804.	0.8	40
58	Phase transitions at zero temperature in the dipolar lattice gas. The Journal of Physical Chemistry, 1992, 96, 1951-1956.	2.9	19
59	Is aluminum-argon (AlAr12) icosahedral?. The Journal of Physical Chemistry, 1992, 96, 5325-5331.	2.9	7
60	Domain energies of the dipolar lattice gas. The Journal of Physical Chemistry, 1992, 96, 1938-1950.	2.9	36
61	Domain-array melting in the dipolar lattice gas. Physical Review B, 1992, 46, 5783-5786.	1.1	44
62	Electronic spectra of NaAr4and NaAr6: Isomerization and melting. Journal of Chemical Physics, 1992, 96, 7977-7991.	1.2	25
63	Accurate non-local electronâ€"argon pseudopotential for condensed phase simulation. Chemical Physics Letters, 1991, 184, 571-578.	1.2	8
64	Multiparticle Monte Carlo moves: Algorithm for solids with free-energy determination. Computer Physics Communications, 1990, 59, 463-470.	3.0	4
65	Multiconfigurational electronic wave functions without a reference configuration: Analysis of a simulated annealing strategy. Journal of Chemical Physics, 1990, 93, 7201-7212.	1.2	7
66	Monte Carlo study of fluidâ€"plastic crystal coexistence in hard dumbbells. Journal of Chemical Physics, 1990, 93, 1278-1286.	1.2	54
67	Electronic energy shifts of a sodium atom in argon clusters by simulated annealing. Journal of Chemical Physics, 1990, 93, 7187-7200.	1.2	45
68	Incorporating advantages of timeâ€dependent dynamics in timeâ€independent collision methods: Early asymptotic analysis. Journal of Chemical Physics, 1989, 91, 240-249.	1.2	10
69	Stochastic molecular dynamics study of cyclohexane isomerization. The Journal of Physical Chemistry, 1988, 92, 3261-3267.	2.9	74
70	A density functional treatment of the hard dumbbell freezing transition. Journal of Chemical Physics, 1987, 87, 4853-4858.	1.2	73
71	Multichannel quantum theory for propagation of second order transition amplitudes. Journal of Chemical Physics, 1987, 87, 4762-4778.	1.2	33
72	Nonadiabatic effects on the photodissociation of diatomic molecules to open-shell atoms. The Journal of Physical Chemistry, 1987, 91, 5402-5409.	2.9	5

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73	Orientation, alignment, and hyperfine effects on dissociation of diatomic molecules to open shell atoms. Journal of Chemical Physics, 1986, 84, 3762-3770.	1.2	25
74	Non-adiabatic effects on the photodissociation of diatomic molecules to open-shell atoms. Resonances, polarizations and angular distributions for the CH+ model systems. Faraday Discussions of the Chemical Society, 1986, 82, 51.	2.2	20
75	RISM calculation of the activation barrier for isomerization of solvated cyclohexane. The Journal of Physical Chemistry, 1986, 90, 6015-6017.	2.9	21
76	Density functional theory of nonuniform polyatomic systems. I. General formulation. Journal of Chemical Physics, 1986, 85, 5971-5976.	1.2	358
77	Density functional theory of nonuniform polyatomic systems. II. Rational closures for integral equations. Journal of Chemical Physics, 1986, 85, 5977-5982.	1.2	223
78	Free energy functions in the extended RISM approximation. Molecular Physics, 1985, 55, 621-625.	0.8	331
79	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.	1.2	36
80	Photodissociation of homonuclear diatomics: Fine structure cross sections for Na2(X1Î£g+) â†' Na(2S1/2) +		