William C Swope

List of Publications by Year
in descending order

60 papers	9,750 citations	147801 31 h-index	128289 60 g-index
60 all docs	60 docs citations	60 times ranked	8950 citing authors

#	Article	IF	Citations
1	A computer simulation method for the calculation of equilibrium constants for the formation of physical clusters of molecules: Application to small water clusters. Journal of Chemical Physics, 1982, 76, 637-649.	3.0	3,203
2	Development of an improved four-site water model for biomolecular simulations: TIP4P-Ew. Journal of Chemical Physics, 2004, 120, 9665-9678.	3.0	1,747
3	Extremely precise free energy calculations of amino acid side chain analogs: Comparison of common molecular mechanics force fields for proteins. Journal of Chemical Physics, 2003, 119, 5740-5761.	3.0	611
4	Use of the Weighted Histogram Analysis Method for the Analysis of Simulated and Parallel Tempering Simulations. Journal of Chemical Theory and Computation, 2007, 3, 26-41.	5.3	416
5	Describing Protein Folding Kinetics by Molecular Dynamics Simulations. 1. Theory. Journal of Physical Chemistry B, 2004, 108, 6571-6581.	2.6	391
6	The role of long ranged forces in determining the structure and properties of liquid water. Journal of Chemical Physics, 1983, 79, 4576-4584.	3.0	340
7	Understanding folding and design: Replica-exchange simulations of "Trp-cage" miniproteins. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 7587-7592.	7.1	331
8	106-particle molecular-dynamics study of homogeneous nucleation of crystals in a supercooled atomic liquid. Physical Review B, 1990, 41, 7042-7054.	3.2	275
9	The Reaction Mechanism for the Organocatalytic Ring-Opening Polymerization of <scp>l</scp>-Lactide Using a Guanidine-Based Catalyst: Hydrogen-Bonded or Covalently Bound?. Journal of the American Chemical Society, 2008, 130, 6749-6754.	13.7	230
10	Longâ€Time Protein Folding Dynamics from Shortâ€Time Molecular Dynamics Simulations. Multiscale Modeling and Simulation, 2006, 5, 1214-1226.	1.6	204
11	Building a More Predictive Protein Force Field: A Systematic and Reproducible Route to AMBER-FB15. Journal of Physical Chemistry B, 2017, 121, 4023-4039.	2.6	192
12	Describing Protein Folding Kinetics by Molecular Dynamics Simulations. 2. Example Applications to Alanine Dipeptide and a Î²-Hairpin Peptide. Journal of Physical Chemistry B, 2004, 108, 6582-6594.	2.6	171
13	Heterogeneous Folding of the trpzip Hairpin: Full Atom Simulation and Experiment. Journal of Molecular Biology, 2004, 336, 241-251.	4.2	165
14	Computer Simulation Study of the Melting Transition in Two Dimensions. Physical Review Letters, 1996, 76, 255-258.	7.8	103
15	Characterization of the TIP4P-Ew water model: Vapor pressure and boiling point. Journal of Chemical Physics, 2005, 123, 194504.	3.0	103
16	Derivation of Fixed Partial Charges for Amino Acids Accommodating a Specific Water Model and Implicit Polarization. Journal of Physical Chemistry B, 2013, 117, 2328-2338.	2.6	95
17	ff14ipq: A Self-Consistent Force Field for Condensed-Phase Simulations of Proteins. Journal of Chemical Theory and Computation, 2014, 10, 4515-4534.	5.3	87
18	Diatomic sulfur: Low lying bound molecular electronic states of S2. Journal of Chemical Physics, 1979, 70, 947.	3.0	76

#	Article	IF	Citations
19	The H3+ potential surface. Journal of Chemical Physics, 1979, 70, 1.	3.0	70
20	Observation of a two-stage melting transition in two dimensions. Physical Review E, 1996, 53, 3794-3803.	2.1	59
21	Toward a Standard Protocol for Micelle Simulation. Journal of Physical Chemistry B, 2016, 120, 6337-6351.	2.6	55
22	The uncoupled symmetric stretching frequency of H3+. Journal of Chemical Physics, 1978, 68, 3951-3952.	3.0	52
23	Thermodynamics, statistical thermodynamics, and computer simulation of crystals with vacancies and interstitials. Physical Review A, 1992, 46, 4539-4548.	2.5	50
24	Sulfur oxide: Lowâ€lying bound molecular electronic states of SO. Journal of Chemical Physics, 1979, 71, 3761-3769.	3.0	48
25	Absence of reptation in the high-temperature folding of the trpzip2 Î²-hairpin peptide. Journal of Chemical Physics, 2006, 124, 141102.	3.0	44
26	Accounting for Polarization Cost When Using Fixed Charge Force Fields. I. Method for Computing Energy. Journal of Physical Chemistry B, 2010, 114, 8621-8630.	2.6	43
27	Toward biodegradable nanogel star polymers via organocatalytic ROP. Chemical Communications, 2012, 48, 6163.	4.1	39
28	Blue Matter: Strong Scaling of Molecular Dynamics on Blue Gene/L. Lecture Notes in Computer Science, 2006, , 846-854.	1.3	38
29	Model organometallic systems. The interaction of 2S beryllium(1+) ion, 1S beryllium, and 3P beryllium atoms with acetylene and ethylene. Journal of the American Chemical Society, 1976, 98, 7962-7967.	13.7	34
30	Laser drilling with focused Gaussian beams. Journal of Applied Physics, 1992, 72, 3686-3696.	2.5	32
31	A computer simulation method for the calculation of chemical potentials of liquids and solids using the bicanonical ensemble. Journal of Chemical Physics, 1995, 102, 2851-2863.	3.0	32
32	Observation of Noncooperative Folding Thermodynamics in Simulations of 1BBL. Biophysical Journal, 2008, 94, 4837-4846.	0.5	32
33	Accounting for Polarization Cost When Using Fixed Charge Force Fields. II. Method and Application for Computing Effect of Polarization Cost on Free Energy of Hydration. Journal of Physical Chemistry B, 2010, 114, 8631-8645.	2.6	32
34	Model studies of Ï€-bonded organometallic systems Mn-C2H2 and Mn-C2H4. Molecular Physics, 1977, 34, 1037-1048.	1.7	30
35	Free energy perturbation calculations involving potential function changes. Journal of Computational Chemistry, 1992, 13, 362-370.	3.3	29
36	Comparison of computational approaches for predicting the effects of missense mutations on p53 function. Journal of Molecular Graphics and Modelling, 2009, 27, 978-982.	2.4	26

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37	Correlation of early orientational ordering of engineered Î»6â€“85 structure with kinetics and thermodynamics. Chemical Physics, 2006, 323, 45-53.	1.9	22
38	Challenge to Reconcile Experimental Micellar Properties of the CnEm Nonionic Surfactant Family. Journal of Physical Chemistry B, 2019, 123, 1696-1707.	2.6	22
39	QM/MM-Based Fitting of Atomic Polarizabilities for Use in Condensed-Phase Biomolecular Simulation. Journal of Chemical Theory and Computation, 2012, 8, 3839-3853.	5.3	20
40	Alternative expressions for energies and forces due to angle bending and torsional energy. Journal of Computational Chemistry, 1992, 13, 585-594.	3.3	19
41	Molecular Dynamics Simulations of Star Polymeric Molecules with Diblock Arms, a Comparative Study. Journal of Chemical Theory and Computation, 2012, 8, 3733-3749.	5.3	18
42	Kinetic Computational Alanine Scanning: Application to p53 Oligomerization. Journal of Molecular Biology, 2006, 357, 1039-1049.	4.2	17
43	Reducing Lambda Repressor to the Core. Journal of Physical Chemistry B, 2011, 115, 2090-2096.	2.6	16
44	BERKELEY: An â€œopen endedâ€•Configuration Interaction (CI) program designed for minicomputers. Journal of Computational Physics, 1978, 26, 243-251.	3.8	14
45	Interfacial Fluctuations of Block Copolymers:â€‰ A Coarse-Grain Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2007, 111, 13734-13742.	2.6	14
46	Model for the Simulation of the C_nE_m Nonionic Surfactant Family Derived from Recent Experimental Results. Journal of Physical Chemistry B, 2020, 124, 9701-9721.	2.6	12
47	Role of Hydrophilicity and Length of Diblock Arms for Determining Star Polymer Physical Properties. Journal of Physical Chemistry B, 2015, 119, 944-957.	2.6	10
48	Water soluble, biodegradable amphiphilic polymeric nanoparticles and the molecular environment of hydrophobic encapsulates: Consistency between simulation and experiment. Polymer, 2015, 79, 255-261.	3.8	10
49	What can digitisation do for formulated product innovation and development?. Polymer International, 2021, 70, 248-255.	3.1	10
50	Structural transition of nanogel star polymers with pH by controlling PEGMA interactions with acid or base copolymers. Molecular Physics, 2016, 114, 3221-3231.	1.7	9
51	A QM/MM Derived Polarizable Water Model for Molecular Simulation. Molecules, 2018, 23, 3131.	3.8	9
52	The Role of Chemical Heterogeneity in Surfactant Adsorption at Solidâ€“Liquid Interfaces. Journal of Chemical Theory and Computation, 2020, 16, 7135-7147.	5.3	8
53	Effect of Hydrophobic Core Topology and Composition on the Structure and Kinetics of Star Polymers: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2017, 121, 2902-2918.	2.6	7
54	Influence of Solvent on the Drug-Loading Process of Amphiphilic Nanogel Star Polymers. Journal of Physical Chemistry B, 2018, 122, 5356-5367.	2.6	7

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55	Spatial Distribution of Hydrophobic Drugs in Model Nanogel-Core Star Polymers. Macromolecules, 2017, 50, 9702-9712.	4.8	6
56	Efficient Algorithm for the Topological Characterization of Worm-like and Branched Micelle Structures from Simulations. Journal of Chemical Theory and Computation, 2020, 16, 4588-4598.	5.3	5
57	Simulation and Experiments To Identify Factors Allowing Synthetic Control of Structural Features of Polymeric Nanoparticles. Journal of Physical Chemistry B, 2016, 120, 7546-7568.	2.6	4
58	A harmonic oscillator model for the magnetic properties of a closed-shell system. Molecular Physics, 1979, 38, 287-298.	1.7	3
59	Chapter 6 Blue Matter: Scaling of N-Body Simulations to One Atom per Node. Current Topics in Membranes, 2008, 60, 159-180.	0.9	2
60	The effect of workstation technology on methods in drug design and discovery. Journal of Computer - Aided Molecular Design, 1993, 1, 359-370.	1.0	1