M Scott Shell

List of Publications by Year
in descending order

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63 papers	4,411 citations	159358 30 h-index	110170 64 g-index
66 all docs	66 docs citations	66 times ranked	3949 citing authors

#	Article	IF	Citations
1	The Protein Folding Problem. Annual Review of Biophysics, 2008, 37, 289-316.	4.5	916
2	The relative entropy is fundamental to multiscale and inverse thermodynamic problems. Journal of Chemical Physics, 2008, 129, 144108.	1.2	483
3	Molecular structural order and anomalies in liquid silica. Physical Review E, 2002, 66, 011202.	0.8	215
4	Coarse-graining errors and numerical optimization using a relative entropy framework. Journal of Chemical Physics, 2011, 134, 094112.	1.2	211
5	Generalization of the Wang-Landau method for off-lattice simulations. Physical Review E, 2002, 66, 056703.	0.8	209
6	The search for the hydrophobic force law. Faraday Discussions, 2010, 146, 299.	1.6	154
7	A Test on Peptide Stability of AMBER Force Fields with Implicit Solvation. Journal of Physical Chemistry B, 2008, 112, 6878-6886.	1.2	130
8	An improved Monte Carlo method for direct calculation of the density of states. Journal of Chemical Physics, 2003, 119, 9406-9411.	1.2	128
9	Anomalous waterlike behavior in spherically-symmetric water models optimized with the relative entropy. Physical Chemistry Chemical Physics, 2009, 11, 1901.	1.3	114
10	The impact of resolution upon entropy and information in coarse-grained models. Journal of Chemical Physics, 2015, 143, 243104.	1.2	106
11	Surface chemical heterogeneity modulates silica surface hydration. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 2890-2895.	3.3	105
12	A New Multiscale Algorithm and Its Application to Coarse-Grained Peptide Models for Self-Assembly. Journal of Physical Chemistry B, 2012, 116, 8383-8393.	1.2	102
13	Coarse-grained models using local-density potentials optimized with the relative entropy: Application to implicit solvation. Journal of Chemical Physics, 2016, 145, 034109.	1.2	83
14	Relative entropy as a universal metric for multiscale errors. Physical Review E, 2010, 81, 060104.	0.8	82
15	Designing Solute-Tailored Selectivity in Membranes: Perspectives for Water Reuse and Resource Recovery. ACS Macro Letters, 2020, 9, 1709-1717.	2.3	62
16	Development of an optimized activatable MMP-14 targeted SPECT imaging probe. Bioorganic and Medicinal Chemistry, 2009, 17, 653-659.	1.4	61
17	Systematic coarse-graining of potential energy landscapes and dynamics in liquids. Journal of Chemical Physics, 2012, 137, 084503.	1.2	57
18	Transferable Coarse-Grained Models of Liquidâ€“Liquid Equilibrium Using Local Density Potentials Optimized with the Relative Entropy. Journal of Physical Chemistry B, 2018, 122, 5678-5693.	1.2	57

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19	Water Structure and Properties at Hydrophilic and Hydrophobic Surfaces. Annual Review of Chemical and Biomolecular Engineering, 2020, 11, 523-557.	3.3	57
20	Electric Double-Layer Structure in Primitive Model Electrolytes: Comparing Molecular Dynamics with Local-Density Approximations. Langmuir, 2015, 31, 3553-3562.	1.6	55
21	A test of systematic coarse-graining of molecular dynamics simulations: Thermodynamic properties. Journal of Chemical Physics, 2012, 137, 164106.	1.2	54
22	Blind Test of Physics-Based Prediction of Protein Structures. Biophysical Journal, 2009, 96, 917-924.	0.2	46
23	Computational discovery of chemically patterned surfaces that effect unique hydration water dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 8093-8098.	3.3	43
24	An Information-Theory-Based Approach for Optimal Model Reduction of Biomolecules. Journal of Chemical Theory and Computation, 2020, 16, 6795-6813.	2.3	41
25	Model Energy Landscapes. Journal of Physical Chemistry B, 2003, 107, 14434-14442.	1.2	40
26	Convergence and Heterogeneity in Peptide Folding with Replica Exchange Molecular Dynamics. Journal of Chemical Theory and Computation, 2009, 5, 2062-2073.	2.3	40
27	Unraveling Hydrophobic Interactions at the Molecular Scale Using Force Spectroscopy and Molecular Dynamics Simulations. ACS Nano, 2017, 11, 2586-2597.	7.3	37
28	Flat-Histogram Dynamics and Optimization in Density of States Simulations of Fluidsâ€. Journal of Physical Chemistry B, 2004, 108, 19748-19755.	1.2	34
29	Hybrid molecular-continuum simulations using smoothed dissipative particle dynamics. Journal of Chemical Physics, 2015, 142, 044101.	1.2	32
30	Predicting Peptide Structures in Native Proteins from Physical Simulations of Fragments. PLoS Computational Biology, 2009, 5, e1000281.	1.5	30
31	Exploring the landscape of model representations. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 24061-24068.	3.3	29
32	Are AMBER Force Fields and Implicit Solvation Models Additive? A Folding Study with a Balanced Peptide Test Set. Journal of Chemical Theory and Computation, 2016, 12, 5631-5642.	2.3	26
33	Evaporation-induced assembly of colloidal crystals. Journal of Chemical Physics, 2018, 149, 094901.	1.2	26
34	Saddles in the Energy Landscape: Extensivity and Thermodynamic Formalism. Physical Review Letters, 2004, 92, 035506.	2.9	25
35	Learning composition-transferable coarse-grained models: Designing external potential ensembles to maximize thermodynamic information. Journal of Chemical Physics, 2020, 153, 154116.	1.2	25
36	Universal Gas Adsorption Mechanism for Flat Nanobubble Morphologies. Physical Review Letters, 2020, 125, 146101.	2.9	24

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37	Affinity of small-molecule solutes to hydrophobic, hydrophilic, and chemically patterned interfaces in aqueous solution. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	24
38	A hybrid, bottom-up, structurally accurate, GoÂ¯-like coarse-grained protein model. Journal of Chemical Physics, 2019, 151, 044111.	1.2	23
39	End-to-End Distance Probability Distributions of Dilute Poly(ethylene oxide) in Aqueous Solution. Journal of the American Chemical Society, 2020, 142, 19631-19641.	6.6	22
40	Molecularly Informed Field Theories from Bottom-up Coarse-Graining. ACS Macro Letters, 2021, 10, 576-583.	2.3	22
41	Inherent-Structure View of Self-Diffusion in Liquids. Journal of Physical Chemistry B, 2004, 108, 6772-6777.	1.2	21
42	Length-scale crossover of the hydrophobic interaction in a coarse-grained water model. Physical Review E, 2013, 88, 052313.	0.8	21
43	A microcanonical approach to temperature-transferable coarse-grained models using the relative entropy. Journal of Chemical Physics, 2021, 155, 094102.	1.2	21
44	Thermodynamics and the glass transition in model energy landscapes. Physical Review E, 2004, 69, 051102.	0.8	20
45	Tetrahedrality and structural order for hydrophobic interactions in a coarse-grained water model. Physical Review E, 2014, 89, 022140.	0.8	20
46	Evidence for Entropically Controlled Interfacial Hydration in Mesoporous Organosilicas. Journal of the American Chemical Society, 2022, 144, 1766-1777.	6.6	20
47	Transferability of Local Density-Assisted Implicit Solvation Models for Homogeneous Fluid Mixtures. Journal of Chemical Theory and Computation, 2019, 15, 2881-2895.	2.3	19
48	Multiscale simulation of ideal mixtures using smoothed dissipative particle dynamics. Journal of Chemical Physics, 2016, 144, 084115.	1.2	17
49	Decoding signatures of structure, bulk thermodynamics, and solvation in three-body angle distributions of rigid water models. Journal of Chemical Physics, 2019, 151, 094501.	1.2	16
50	Two-dimensional replica exchange approach for peptideâ€“peptide interactions. Journal of Chemical Physics, 2011, 134, 064112.	1.2	15
51	Charge Effects on the Fibril-Forming Peptide KTVIIE: A Two-Dimensional Replica Exchange Simulation Study. Biophysical Journal, 2012, 102, 1952-1960.	0.2	14
52	Entropic (de)stabilization of surface-bound peptides conjugated with polymers. Journal of Chemical Physics, 2015, 143, 243103.	1.2	12
53	Coupling discrete and continuum concentration particle models for multiscale and hybrid molecular-continuum simulations. Journal of Chemical Physics, 2017, 147, 234112.	1.2	12
54	Extrapolation and interpolation strategies for efficiently estimating structural observables as a function of temperature and density. Journal of Chemical Physics, 2020, 153, 144101.	1.2	12

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55	Computational characterization of the sequence landscape in simple protein alphabets. Proteins: Structure, Function and Bioinformatics, 2005, 62, 232-243.	1.5	11
56	Can Peptide Folding Simulations Provide Predictive Information for Aggregation Propensity?. Journal of Physical Chemistry B, 2010, 114, 11899-11908.	1.2	11
57	Sequence Modulates Polypeptoid Hydration Water Structure and Dynamics. Biomacromolecules, 2022, 23, 1745-1756.	2.6	11
58	Quantifying Polypeptoid Conformational Landscapes through Integrated Experiment and Simulation. Macromolecules, 2021, 54, 5011-5021.	2.2	9
59	Smoothing Protein Energy Landscapes by Integrating Folding Models with Structure Prediction. Biophysical Journal, 2011, 101, 2251-2259.	0.2	8
60	A replica-exchange approach to computing peptide conformational free energies. Molecular Simulation, 2010, 36, 505-515.	0.9	3
61	Can Simple Interaction Models Explain Sequence-Dependent Effects in Peptide Homodimerization?. Journal of Physical Chemistry B, 2017, 121, 5928-5943.	1.2	2
62	Novel Computational Probes of Diffusive Motion. Journal of Physical Chemistry B, 2005, 109, 21329-21333.	1.2	1
63	Peptide binding landscapes: Specificity and homophilicity across sequence space in a lattice model. Physical Review E, 2016, 94, 042405.	0.8	0