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	Evidence for Entropically Controlled Interfacial Hydration in Mesoporous Organosilicas. Journal of the American Chemical Society, 2022, 144, 1766-1777.	6.6	20
2	Sequence Modulates Polypeptoid Hydration Water Structure and Dynamics. Biomacromolecules, 2022, 23, 1745-1756.	2.6	11
3	Molecularly Informed Field Theories from Bottom-up Coarse-Graining. ACS Macro Letters, 2021, 10, 576-583.	2.3	22
4	Quantifying Polypeptoid Conformational Landscapes through Integrated Experiment and Simulation. Macromolecules, 2021, 54, 5011-5021.	2.2	9
5	A microcanonical approach to temperature-transferable coarse-grained models using the relative entropy. Journal of Chemical Physics, 2021, 155, 094102.	1.2	21
6	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
7	Universal Gas Adsorption Mechanism for Flat Nanobubble Morphologies. Physical Review Letters, 2020, 125, 146101.	2.9	24
8	An Information-Theory-Based Approach for Optimal Model Reduction of Biomolecules. Journal of Chemical Theory and Computation, 2020, 16, 6795-6813.	2.3	41
9	Learning composition-transferable coarse-grained models: Designing external potential ensembles to maximize thermodynamic information. Journal of Chemical Physics, 2020, 153, 154116.	1.2	25
10	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
11	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
12	Designing Solute-Tailored Selectivity in Membranes: Perspectives for Water Reuse and Resource Recovery. ACS Macro Letters, 2020, 9, 1709-1717.	2.3	62
13	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
14	Water Structure and Properties at Hydrophilic and Hydrophobic Surfaces. Annual Review of Chemical and Biomolecular Engineering, 2020, 11, 523-557.	3.3	57
15	A hybrid, bottom-up, structurally accurate, GoÂ¯-like coarse-grained protein model. Journal of Chemical Physics, 2019, 151, 044111.	1.2	23
16	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
17	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
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	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
20	Evaporation-induced assembly of colloidal crystals. Journal of Chemical Physics, 2018, 149, 094901.	1.2	26
21	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
22	Unraveling Hydrophobic Interactions at the Molecular Scale Using Force Spectroscopy and Molecular Dynamics Simulations. ACS Nano, 2017, 11, 2586-2597.	7.3	37
23	Can Simple Interaction Models Explain Sequence-Dependent Effects in Peptide Homodimerization?. Journal of Physical Chemistry B, 2017, 121, 5928-5943.	1.2	2
24	Coupling discrete and continuum concentration particle models for multiscale and hybrid molecular-continuum simulations. Journal of Chemical Physics, 2017, 147, 234112.	1.2	12
25	Multiscale simulation of ideal mixtures using smoothed dissipative particle dynamics. Journal of Chemical Physics, 2016, 144, 084115.	1.2	17
26	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
27	Peptide binding landscapes: Specificity and homophilicity across sequence space in a lattice model. Physical Review E, 2016, 94, 042405.	0.8	0
28	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
29	Entropic (de)stabilization of surface-bound peptides conjugated with polymers. Journal of Chemical Physics, 2015, 143, 243103.	1.2	12
30	The impact of resolution upon entropy and information in coarse-grained models. Journal of Chemical Physics, 2015, 143, 243104.	1.2	106
31	Hybrid molecular-continuum simulations using smoothed dissipative particle dynamics. Journal of Chemical Physics, 2015, 142, 044101.	1.2	32
32	Electric Double-Layer Structure in Primitive Model Electrolytes: Comparing Molecular Dynamics with Local-Density Approximations. Langmuir, 2015, 31, 3553-3562.	1.6	55
33	Tetrahedrality and structural order for hydrophobic interactions in a coarse-grained water model. Physical Review E, 2014, 89, 022140.	0.8	20
34	Length-scale crossover of the hydrophobic interaction in a coarse-grained water model. Physical Review E, 2013, 88, 052313.	0.8	21
35	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
36	A test of systematic coarse-graining of molecular dynamics simulations: Thermodynamic properties. Journal of Chemical Physics, 2012, 137, 164106.	1.2	54

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37	Systematic coarse-graining of potential energy landscapes and dynamics in liquids. Journal of Chemical Physics, 2012, 137, 084503.	1.2	57
38	Charge Effects on the Fibril-Forming Peptide KTVIIE: A Two-Dimensional Replica Exchange Simulation Study. Biophysical Journal, 2012, 102, 1952-1960.	0.2	14
39	Smoothing Protein Energy Landscapes by Integrating Folding Models with Structure Prediction. Biophysical Journal, 2011, 101, 2251-2259.	0.2	8
40	Coarse-graining errors and numerical optimization using a relative entropy framework. Journal of Chemical Physics, 2011, 134, 094112.	1.2	211
41	Two-dimensional replica exchange approach for peptideâ€“peptide interactions. Journal of Chemical Physics, 2011, 134, 064112.	1.2	15
42	Can Peptide Folding Simulations Provide Predictive Information for Aggregation Propensity?. Journal of Physical Chemistry B, 2010, 114, 11899-11908.	1.2	11
43	Relative entropy as a universal metric for multiscale errors. Physical Review E, 2010, 81, 060104.	0.8	82
44	The search for the hydrophobic force law. Faraday Discussions, 2010, 146, 299.	1.6	154
45	A replica-exchange approach to computing peptide conformational free energies. Molecular Simulation, 2010, 36, 505-515.	0.9	3
46	Predicting Peptide Structures in Native Proteins from Physical Simulations of Fragments. PLoS Computational Biology, 2009, 5, e1000281.	1.5	30
47	Development of an optimized activatable MMP-14 targeted SPECT imaging probe. Bioorganic and Medicinal Chemistry, 2009, 17, 653-659.	1.4	61
48	Convergence and Heterogeneity in Peptide Folding with Replica Exchange Molecular Dynamics. Journal of Chemical Theory and Computation, 2009, 5, 2062-2073.	2.3	40
49	Blind Test of Physics-Based Prediction of Protein Structures. Biophysical Journal, 2009, 96, 917-924.	0.2	46
50	Anomalous waterlike behavior in spherically-symmetric water models optimized with the relative entropy. Physical Chemistry Chemical Physics, 2009, 11, 1901.	1.3	114
51	The Protein Folding Problem. Annual Review of Biophysics, 2008, 37, 289-316.	4.5	916
52	The relative entropy is fundamental to multiscale and inverse thermodynamic problems. Journal of Chemical Physics, 2008, 129, 144108.	1.2	483
53	A Test on Peptide Stability of AMBER Force Fields with Implicit Solvation. Journal of Physical Chemistry B, 2008, 112, 6878-6886.	1.2	130
54	Computational characterization of the sequence landscape in simple protein alphabets. Proteins: Structure, Function and Bioinformatics, 2005, 62, 232-243.	1.5	11

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55	Novel Computational Probes of Diffusive Motion. Journal of Physical Chemistry B, 2005, 109, 21329-21333.	1.2	1
56	Saddles in the Energy Landscape: Extensivity and Thermodynamic Formalism. Physical Review Letters, 2004, 92, 035506.	2.9	25
57	Flat-Histogram Dynamics and Optimization in Density of States Simulations of Fluidsâ€. Journal of Physical Chemistry B, 2004, 108, 19748-19755.	1.2	34
58	Thermodynamics and the glass transition in model energy landscapes. Physical Review E, 2004, 69, 051102.	0.8	20
59	Inherent-Structure View of Self-Diffusion in Liquids. Journal of Physical Chemistry B, 2004, 108, 6772-6777.	1.2	21
60	Model Energy Landscapes. Journal of Physical Chemistry B, 2003, 107, 14434-14442.	1.2	40
61	An improved Monte Carlo method for direct calculation of the density of states. Journal of Chemical Physics, 2003, 119, 9406-9411.	1.2	128
62	Generalization of the Wang-Landau method for off-lattice simulations. Physical Review E, 2002, 66, 056703.	0.8	209
63	Molecular structural order and anomalies in liquid silica. Physical Review E, 2002, 66, 011202.	0.8	215