Charusita Chakravarty

List of Publications by Year
in descending order

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96	3,452	117453	155451
papers	citations	34 h-index	55 g-index

100	100	100	2308
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Hydration Behavior along the Folding Pathways of Trpzip4, Trpzip5 and Trpzip6. Journal of Physical Chemistry B, 2018, 122, 1560-1572.	1.2	6
2	Probing the triplet correlation function in liquid water by experiments and molecular simulations. Physical Chemistry Chemical Physics, 2017, 19, 3265-3278.	1.3	14
3	Thermodynamic regimes over which homologous alkane fluids can be treated as simple liquids. Journal of Molecular Liquids, 2017, 231, 106-115.	2.3	6
4	Concentration-dependent structure and dynamics of aqueous LiCl solutions: A molecular dynamics study. Journal of Molecular Liquids, 2017, 225, 240-250.	2.3	15
5	Solvation of LiCl in model liquids with high to low hydrogen bond strengths. Journal of Chemical Physics, 2017, 146, 184503.	1.2	3
6	The sensitivity of folding free energy landscapes of trpzips to mutations in the hydrophobic core. Physical Chemistry Chemical Physics, 2017, 19, 22813-22825.	1.3	5
7	Thiolated gold nanoparticle solvation in near-critical fluids: The role of density, temperature, and topology. Journal of Chemical Physics, 2017, 146, 174902.	1.2	5
8	Water: A Tale of Two Liquids. Chemical Reviews, 2016, 116, 7463-7500.	23.0	627
9	Comparison of liquid-state anomalies in Stillinger-Weber models of water, silicon, and germanium. Journal of Chemical Physics, 2016, 145, 214502.	1.2	37
10	Effective interactions between nanoparticles: Creating temperature-independent solvation environments for self-assembly. Journal of Chemical Physics, 2016, 144, 244901.	1.2	13
11	Tuning the tetrahedrality of the hydrogen-bonded network of water: Comparison of the effects of pressure and added salts. Journal of Chemical Physics, 2016, 144, 234509.	1.2	7
12	Relationship between the line of density anomaly and the lines of melting, crystallization, cavitation, and liquid spinodal in coarse-grained water models. Journal of Chemical Physics, 2016, 144, 234507.	1.2	32
13	Comparison of hydration behavior and conformational preferences of the Trp-cage mini-protein in different rigid-body water models. Physical Chemistry Chemical Physics, 2016, 18, 32796-32813.	1.3	16
14	Sensitivity of Protein Glass Transition to the Choice of Water Model. Journal of Chemical Theory and Computation, 2016, 12, 5643-5655.	2.3	16
15	Water-like Anomalies and Phase Behavior of a Pair Potential that Stabilizes Diamond. Journal of Physical Chemistry B, 2016, 120, 1649-1659.	1.2	10
16	Excess entropy and crystallization in Stillinger-Weber and Lennard-Jones fluids. Journal of Chemical Physics, 2015, 143, 164512.	1.2	34
17	Free Energy Landscapes of Alanine Oligopeptides in Rigid-Body and Hybrid Water Models. Journal of Physical Chemistry B, 2015, 119, 11106-11120.	1.2	6
18	Fluctuation-driven anisotropy in effective pair interactions between nanoparticles: Thiolated gold nanoparticles in ethane. Journal of Chemical Physics, 2014, 141, 154904.	1.2	26

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19	Triplet correlation functions in liquid water. Journal of Chemical Physics, 2014, 141, 174504.	1.2	25
20	Onset of simple liquid behaviour in modified water models. Journal of Chemical Physics, 2014, 140, 164501.	1.2	31
21	Sensitivity of local hydration behaviour and conformational preferences of peptides to choice of water model. Physical Chemistry Chemical Physics, 2014, 16, 10199-10213.	1.3	20
22	Triplet Correlations Dominate the Transition from Simple to Tetrahedral Liquids. Physical Review Letters, 2014, 112, 147801.	2.9	40
23	Water and water-like liquids: relationships between structure, entropy and mobility. Physical Chemistry Chemical Physics, 2013, 15, 14162.	1.3	66
24	Fluctuation-Driven Anisotropic Assembly in Nanoscale Systems. Nano Letters, 2013, 13, 2732-2737.	4.5	57
25	Relating Structure, Entropy, and Energy of Solvation of Nanoscale Solutes: Application to Gold Nanoparticle Dispersions. Journal of Physical Chemistry B, 2012, 116, 13124-13132.	1.2	10
26	Structural correlations and cooperative dynamics in supercooled liquids. Journal of Chemical Physics, 2012, 137, 024508.	1.2	23
27	Relating composition, structural order, entropy and transport in multi-component molten salts. Journal of Chemical Physics, 2012, 136, 144507.	1.2	21
28	Water and other tetrahedral liquids: order, anomalies and solvation. Journal of Physics Condensed Matter, 2012, 24, 284116.	0.7	38
29	Transport in nanoporous zeolites: Relationships between sorbate size, entropy, and diffusivity. Journal of Chemical Physics, 2012, 136, 174510.	1.2	27
30	Structure and transport properties of LiFâ€“BeF2 mixtures: Comparison of rigid and polarizable ion potentials#. Journal of Chemical Sciences, 2012, 124, 261-269.	0.7	15
31	Thermodynamic, Diffusional, and Structural Anomalies in Rigid-Body Water Models. Journal of Physical Chemistry B, 2011, 115, 6935-6945.	1.2	79
32	Energy Landscapes of Quantum Lennard-Jones Solids. Journal of Physical Chemistry A, 2011, 115, 7028-7033.	1.1	7
33	Comparison of Tetrahedral Order, Liquid State Anomalies, and Hydration Behavior of mTIP3P and TIP4P Water Models. Journal of Chemical Theory and Computation, 2011, 7, 3354-3367.	2.3	52
34	Core-softened fluids, water-like anomalies, and the liquid-liquid critical points. Journal of Chemical Physics, 2011, 135, 044517.	1.2	29
35	The Rise and Fall of Anomalies in Tetrahedral Liquids. Journal of Statistical Physics, 2011, 145, 293-312.	0.5	67
36	Excess entropy scaling of transport properties in network-forming ionic melts (SiO2 and BeF2). Journal of Chemical Physics, 2011, 134, 014502.	1.2	40

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37	Interplay between multiple length and time scales in complex chemical systems. Journal of Chemical Sciences, 2010, 122, 459-470.	0.7	13
38	Entropy, diffusivity and the energy landscape of a waterlike fluid. Journal of Chemical Physics, 2010, 132, 234509.	1.2	40
39	Tetrahedral order, pair correlation entropy, and waterlike liquid state anomalies: Comparison of GeO2 with BeF2, SiO2, and H2O. Journal of Chemical Physics, 2010, 132, 234507.	1.2	55
40	Local Order, Energy, and Mobility of Water Molecules in the Hydration Shell of Small Peptides. Journal of Physical Chemistry B, 2010, 114, 651-659.	1.2	52
41	Excess entropy and structural transitions in a two-dimensional square-shoulder fluid. Journal of Chemical Physics, 2010, 132, 074503.	1.2	19
42	Relationship between Structure, Entropy, and Diffusivity in Water and Water-Like Liquids. Journal of Physical Chemistry B, 2010, 114, 6995-7001.	1.2	84
43	Relationship between structure, entropy, and mobility in network-forming ionic melts. Physical Review E, 2009, 79, 030202.	0.8	49
44	Evaluation of collective transport properties of ionic melts from molecular dynamics simulations. Journal of Chemical Sciences, 2009, 121, 913-919.	0.7	4
45	Relationship between crystalline order and melting mechanisms of solids. Indian Journal of Physics, 2009, 83, 65-79.	0.9	3
46	Transport Properties of Tetrahedral, Network-Forming Ionic Melts. Journal of Physical Chemistry B, 2009, 113, 15284-15292.	1.2	37
47	Estimating the entropy of liquids from atomâ€“atom radial distribution functions: silica, beryllium fluoride and water. Molecular Physics, 2008, 106, 1925-1938.	0.8	57
48	Multiple Time Scale Behaviors and Network Dynamics in Liquid Methanol. Journal of Physical Chemistry B, 2008, 112, 9071-9078.	1.2	12
49	Excess entropy scaling of transport properties of Lennard-Jones chains. Journal of Chemical Physics, 2008, 129, 164904.	1.2	94
50	Ionic melts with waterlike anomalies: Thermodynamic properties of liquid BeF2. Journal of Chemical Physics, 2007, 127, 164502.	1.2	46
51	Lindemann measures for the solid-liquid phase transition. Journal of Chemical Physics, 2007, 126, 204508.	1.2	83
52	Determining landscape-based criteria for freezing of liquids. Journal of Chemical Physics, 2007, 126, 244512.	1.2	3
53	Waterlike Structural and Excess Entropy Anomalies in Liquid Beryllium Fluoride. Journal of Physical Chemistry B, 2007, 111, 13294-13300.	1.2	44
54	Entropy, local order, and the freezing transition in Morse liquids. Physical Review E, 2007, 76, 011201.	0.8	32

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55	Entropy, diffusivity, and structural order in liquids with waterlike anomalies. Journal of Chemical Physics, 2006, 125, 204501.	1.2	176
56	Effect of Ionic Solutes on the Hydrogen Bond Network Dynamics of Water:Â Power Spectral Analysis of Aqueous NaCl Solutions. Journal of Physical Chemistry B, 2006, 110, 8422-8431.	1.2	34
57	Diffusional anomaly and network dynamics in liquid silica. Journal of Chemical Physics, 2006, 125, 044705.	1.2	37
58	Spectral characterization of hydrogen bond network dynamics in water. Journal of Chemical Physics, 2006, 125, 074508.	1.2	10
59	Diffusivity, excess entropy, and the potential-energy landscape of monatomic liquids. Journal of Chemical Physics, 2006, 124, 014507.	1.2	39
60	Generating inherent structures of liquids: Comparison of local minimization algorithms. Journal of Chemical Physics, 2005, 123, 206101.	1.2	13
61	Spectral signatures of the diffusional anomaly in water. Journal of Chemical Physics, 2005, 122, 104507.	1.2	36
62	Hybrid Monte Carlo implementation of the Fourier path integral algorithm. Journal of Chemical Physics, 2005, 123, 024104.	1.2	6
63	Effect of the Berendsen thermostat on the dynamical properties of water. Molecular Physics, 2004, 102, 681-685.	0.8	40
64	Melting of atomic solids: effect of range and softness of interaction potentials. Molecular Physics, 2004, 102, 909-918.	0.8	11
65	Multiple Time-Scale Behavior of the Hydrogen-Bond Network in Waterâ€. Journal of Physical Chemistry B, 2004, 108, 19607-19613.	1.2	24
66	Signatures of multiple time-scale behaviour in the power spectra of water. Chemical Physics Letters, 2003, 376, 683-689.	1.2	13
67	Quasisaddles of liquids: Computational study of a bulk Lennard-Jones system. Journal of Chemical Physics, 2003, 118, 2342-2348.	1.2	7
68	Melting of 55-atom Morse clusters. Journal of Chemical Physics, 2003, 118, 10671-10682.	1.2	16
69	Path integral simulations of quantum Lennard-Jones solids. Journal of Chemical Physics, 2002, 116, 8938-8947.	1.2	40
70	Instantaneous normal mode analysis of Morse liquids. Journal of Chemical Physics, 2002, 116, 10825-10832.	1.2	10
71	Bond orientational order in atomic clusters. Molecular Physics, 2002, 100, 3777-3780.	0.8	9
72	Potential-Energy Landscapes of Simple Liquids. Physical Review Letters, 2002, 88, 255501.	2.9	26

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73	Diffusional behaviour of simple sorbates in zeolites: effect of anisotropic frameworks and geometrical correlations. Chemical Physics Letters, 2002, 352, 294-300.	1.2	4
74	Diffusional Anisotropy of Simple Sorbates in Silicalite. Journal of Physical Chemistry A, 2001, 105, 5785-5793.	1.1	16
75	Comparison of inherent, instantaneous, and saddle configurations of the bulk Lennard-Jones system. Journal of Chemical Physics, 2001, 115, 8784-8794.	1.2	29
76	Instantaneous Normal Mode Analysis of the Levitation Effect in Zeolites. Journal of Physical Chemistry B, 2000, 104, 709-715.	1.2	16
77	Isothermal-isobaric ensemble simulations of melting in quantum solids. Physical Review B, 1999, 59, 3590-3598.	1.1	16
78	Dynamics of Rare Gases in Zeolites: Instantaneous Normal Mode Analysis. Journal of Physical Chemistry B, 1999, 103, 2740-2748.	1.2	12
79	An ab initio path integral Monte Carlo simulation method for molecules and clusters: Application to Li4 and Li5+. Journal of Chemical Physics, 1998, 108, 8848-8858.	1.2	37
80	Quantum Adsorbates: Helium in Zeolites. , 1998, , 305-308.		0
81	Effects of three-body (Axilrod-Teller) forces on the classical and quantum behavior of rare-gas trimers. Physical Review E, 1997, 56, 363-377.	0.8	30
82	Instantaneous normal mode spectra of quantum clusters. Journal of Chemical Physics, 1997, 106, 5564-5568.	1.2	19
83	Quantum Adsorbates:â€‰ Path Integral Monte Carlo Simulations of Helium in Silicalite. Journal of Physical Chemistry B, 1997, 101, 1878-1883.	1.2	16
84	Path integral simulations of atomic and molecular systems. International Reviews in Physical Chemistry, 1997, 16, 421-444.	0.9	77
85	Cluster analogs of binary isotopic mixtures: Path integral Monte Carlo simulations. Journal of Chemical Physics, 1996, 104, 7223-7232.	1.2	11
86	The kinetics of H2dissociative chemisorption: The role of transients. Journal of Chemical Physics, 1995, 102, 8643-8655.	1.2	10
87	Structure of Binary Quantum Clusters. Physical Review Letters, 1995, 75, 1727-1730.	2.9	22
88	Quantum delocalization and cluster melting. Journal of Chemical Physics, 1995, 103, 10663-10668.	1.2	29
89	Maximal Lyapunov exponent in small atomic clusters. Physical Review E, 1995, 51, 3376-3380.	0.8	50
90	1/fSpectra in Finite Atomic Clusters. Physical Review Letters, 1995, 74, 4181-4184.	2.9	23

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91	Fourier path integral simulations ofpara-H2andortho-D2clusters. Molecular Physics, 1995, 84, 845-852.	0.8	25
92	Melting of neon clusters: Path integral Monte Carlo simulations. Journal of Chemical Physics, 1995, 102, 956-962.	1.2	40
93	STIMULATED EMISSION PUMPING AS A PROBE OF THE OH (X²Î) + Ar INTERMOLECULAR POTENTIAL ENERGY SURFACE. Advanced Series in Physical Chemistry, 1995, , 659-688.	1.5	6
94	Refinement of the OH Aâ€‰2Î£+(v=0)+Ar intermolecular potential energy surface. Journal of Chemical Physics, 1993, 98, 9320-9334.	1.2	52
95	Particle exchange in the Fourier pathâ€integral Monte Carlo technique. Journal of Chemical Physics, 1993, 99, 8038-8043.	1.2	26
96	Stimulated emission pumping of van der Waals vibrations in the ground electronic state of OHî—¸Ar. Chemical Physics Letters, 1991, 178, 301-310.	1.2	63