# Charusita Chakravarty

List of Publications by Year
in descending order

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| 96 | 3,452 | 117625 | 155660 |
|---|---|---|---|
| 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. | 2.6 | 6 |
| 2 | Probing the triplet correlation function in liquid water by experiments and molecular simulations. Physical Chemistry Chemical Physics, 2017, 19, 3265-3278. | 2.8 | 14 |
| 3 | Thermodynamic regimes over which homologous alkane fluids can be treated as simple liquids. Journal of Molecular Liquids, 2017, 231, 106-115. | 4.9 | 6 |
| 4 | Concentration-dependent structure and dynamics of aqueous LiCl solutions: A molecular dynamics study. Journal of Molecular Liquids, 2017, 225, 240-250. | 4.9 | 15 |
| 5 | Solvation of LiCl in model liquids with high to low hydrogen bond strengths. Journal of Chemical Physics, 2017, 146, 184503. | 3.0 | 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. | 2.8 | 5 |
| 7 | Thiolated gold nanoparticle solvation in near-critical fluids: The role of density, temperature, and topology. Journal of Chemical Physics, 2017, 146, 174902. | 3.0 | 5 |
| 8 | Water: A Tale of Two Liquids. Chemical Reviews, 2016, 116, 7463-7500. | 47.7 | 627 |
| 9 | Comparison of liquid-state anomalies in Stillinger-Weber models of water, silicon, and germanium. Journal of Chemical Physics, 2016, 145, 214502. | 3.0 | 37 |
| 10 | Effective interactions between nanoparticles: Creating temperature-independent solvation environments for self-assembly. Journal of Chemical Physics, 2016, 144, 244901. | 3.0 | 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. | 3.0 | 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. | 3.0 | 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. | 2.8 | 16 |
| 14 | Sensitivity of Protein Glass Transition to the Choice of Water Model. Journal of Chemical Theory and Computation, 2016, 12, 5643-5655. | 5.3 | 16 |
| 15 | Water-like Anomalies and Phase Behavior of a Pair Potential that Stabilizes Diamond. Journal of Physical Chemistry B, 2016, 120, 1649-1659. | 2.6 | 10 |
| 16 | Excess entropy and crystallization in Stillinger-Weber and Lennard-Jones fluids. Journal of Chemical Physics, 2015, 143, 164512. | 3.0 | 34 |
| 17 | Free Energy Landscapes of Alanine Oligopeptides in Rigid-Body and Hybrid Water Models. Journal of Physical Chemistry B, 2015, 119, 11106-11120. | 2.6 | 6 |
| 18 | Fluctuation-driven anisotropy in effective pair interactions between nanoparticles: Thiolated gold nanoparticles in ethane. Journal of Chemical Physics, 2014, 141, 154904. | 3.0 | 26 |

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| 19 | Triplet correlation functions in liquid water. Journal of Chemical Physics, 2014, 141, 174504. | 3.0 | 25 |
| 20 | Onset of simple liquid behaviour in modified water models. Journal of Chemical Physics, 2014, 140, 164501. | 3.0 | 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. | 2.8 | 20 |
| 22 | Triplet Correlations Dominate the Transition from Simple to Tetrahedral Liquids. Physical Review Letters, 2014, 112, 147801. | 7.8 | 40 |
| 23 | Water and water-like liquids: relationships between structure, entropy and mobility. Physical Chemistry Chemical Physics, 2013, 15, 14162. | 2.8 | 66 |
| 24 | Fluctuation-Driven Anisotropic Assembly in Nanoscale Systems. Nano Letters, 2013, 13, 2732-2737. | 9.1 | 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. | 2.6 | 10 |
| 26 | Structural correlations and cooperative dynamics in supercooled liquids. Journal of Chemical Physics, 2012, 137, 024508. | 3.0 | 23 |
| 27 | Relating composition, structural order, entropy and transport in multi-component molten salts. Journal of Chemical Physics, 2012, 136, 144507. | 3.0 | 21 |
| 28 | Water and other tetrahedral liquids: order, anomalies and solvation. Journal of Physics Condensed Matter, 2012, 24, 284116. | 1.8 | 38 |
| 29 | Transport in nanoporous zeolites: Relationships between sorbate size, entropy, and diffusivity. Journal of Chemical Physics, 2012, 136, 174510. | 3.0 | 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. | 1.5 | 15 |
| 31 | Thermodynamic, Diffusional, and Structural Anomalies in Rigid-Body Water Models. Journal of Physical Chemistry B, 2011, 115, 6935-6945. | 2.6 | 79 |
| 32 | Energy Landscapes of Quantum Lennard-Jones Solids. Journal of Physical Chemistry A, 2011, 115, 7028-7033. | 2.5 | 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. | 5.3 | 52 |
| 34 | Core-softened fluids, water-like anomalies, and the liquid-liquid critical points. Journal of Chemical Physics, 2011, 135, 044517. | 3.0 | 29 |
| 35 | The Rise and Fall of Anomalies in Tetrahedral Liquids. Journal of Statistical Physics, 2011, 145, 293-312. | 1.2 | 67 |
| 36 | Excess entropy scaling of transport properties in network-forming ionic melts (SiO2 and BeF2). Journal of Chemical Physics, 2011, 134, 014502. | 3.0 | 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. | 1.5 | 13 |
| 38 | Entropy, diffusivity and the energy landscape of a waterlike fluid. Journal of Chemical Physics, 2010, 132, 234509. | 3.0 | 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. | 3.0 | 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. | 2.6 | 52 |
| 41 | Excess entropy and structural transitions in a two-dimensional square-shoulder fluid. Journal of Chemical Physics, 2010, 132, 074503. | 3.0 | 19 |
| 42 | Relationship between Structure, Entropy, and Diffusivity in Water and Water-Like Liquids. Journal of Physical Chemistry B, 2010, 114, 6995-7001. | 2.6 | 84 |
| 43 | Relationship between structure, entropy, and mobility in network-forming ionic melts. Physical Review E, 2009, 79, 030202. | 2.1 | 49 |
| 44 | Evaluation of collective transport properties of ionic melts from molecular dynamics simulations. Journal of Chemical Sciences, 2009, 121, 913-919. | 1.5 | 4 |
| 45 | Relationship between crystalline order and melting mechanisms of solids. Indian Journal of Physics, 2009, 83, 65-79. | 1.8 | 3 |
| 46 | Transport Properties of Tetrahedral, Network-Forming Ionic Melts. Journal of Physical Chemistry B, 2009, 113, 15284-15292. | 2.6 | 37 |
| 47 | Estimating the entropy of liquids from atomâ€“atom radial distribution functions: silica, beryllium fluoride and water. Molecular Physics, 2008, 106, 1925-1938. | 1.7 | 57 |
| 48 | Multiple Time Scale Behaviors and Network Dynamics in Liquid Methanol. Journal of Physical Chemistry B, 2008, 112, 9071-9078. | 2.6 | 12 |
| 49 | Excess entropy scaling of transport properties of Lennard-Jones chains. Journal of Chemical Physics, 2008, 129, 164904. | 3.0 | 94 |
| 50 | Ionic melts with waterlike anomalies: Thermodynamic properties of liquid BeF2. Journal of Chemical Physics, 2007, 127, 164502. | 3.0 | 46 |
| 51 | Lindemann measures for the solid-liquid phase transition. Journal of Chemical Physics, 2007, 126, 204508. | 3.0 | 83 |
| 52 | Determining landscape-based criteria for freezing of liquids. Journal of Chemical Physics, 2007, 126, 244512. | 3.0 | 3 |
| 53 | Waterlike Structural and Excess Entropy Anomalies in Liquid Beryllium Fluoride. Journal of Physical Chemistry B, 2007, 111, 13294-13300. | 2.6 | 44 |
| 54 | Entropy, local order, and the freezing transition in Morse liquids. Physical Review E, 2007, 76, 011201. | 2.1 | 32 |

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| 55 | Entropy, diffusivity, and structural order in liquids with waterlike anomalies. Journal of Chemical Physics, 2006, 125, 204501. | 3.0 | 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. | 2.6 | 34 |
| 57 | Diffusional anomaly and network dynamics in liquid silica. Journal of Chemical Physics, 2006, 125, 044705. | 3.0 | 37 |
| 58 | Spectral characterization of hydrogen bond network dynamics in water. Journal of Chemical Physics, 2006, 125, 074508. | 3.0 | 10 |
| 59 | Diffusivity, excess entropy, and the potential-energy landscape of monatomic liquids. Journal of Chemical Physics, 2006, 124, 014507. | 3.0 | 39 |
| 60 | Generating inherent structures of liquids: Comparison of local minimization algorithms. Journal of Chemical Physics, 2005, 123, 206101. | 3.0 | 13 |
| 61 | Spectral signatures of the diffusional anomaly in water. Journal of Chemical Physics, 2005, 122, 104507. | 3.0 | 36 |
| 62 | Hybrid Monte Carlo implementation of the Fourier path integral algorithm. Journal of Chemical Physics, 2005, 123, 024104. | 3.0 | 6 |
| 63 | Effect of the Berendsen thermostat on the dynamical properties of water. Molecular Physics, 2004, 102, 681-685. | 1.7 | 40 |
| 64 | Melting of atomic solids: effect of range and softness of interaction potentials. Molecular Physics, 2004, 102, 909-918. | 1.7 | 11 |
| 65 | Multiple Time-Scale Behavior of the Hydrogen-Bond Network in Waterâ€. Journal of Physical Chemistry B, 2004, 108, 19607-19613. | 2.6 | 24 |
| 66 | Signatures of multiple time-scale behaviour in the power spectra of water. Chemical Physics Letters, 2003, 376, 683-689. | 2.6 | 13 |
| 67 | Quasisaddles of liquids: Computational study of a bulk Lennard-Jones system. Journal of Chemical Physics, 2003, 118, 2342-2348. | 3.0 | 7 |
| 68 | Melting of 55-atom Morse clusters. Journal of Chemical Physics, 2003, 118, 10671-10682. | 3.0 | 16 |
| 69 | Path integral simulations of quantum Lennard-Jones solids. Journal of Chemical Physics, 2002, 116, 8938-8947. | 3.0 | 40 |
| 70 | Instantaneous normal mode analysis of Morse liquids. Journal of Chemical Physics, 2002, 116, 10825-10832. | 3.0 | 10 |
| 71 | Bond orientational order in atomic clusters. Molecular Physics, 2002, 100, 3777-3780. | 1.7 | 9 |
| 72 | Potential-Energy Landscapes of Simple Liquids. Physical Review Letters, 2002, 88, 255501. | 7.8 | 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. | 2.6 | 4 |
| 74 | Diffusional Anisotropy of Simple Sorbates in Silicalite. Journal of Physical Chemistry A, 2001, 105, 5785-5793. | 2.5 | 16 |
| 75 | Comparison of inherent, instantaneous, and saddle configurations of the bulk Lennard-Jones system. Journal of Chemical Physics, 2001, 115, 8784-8794. | 3.0 | 29 |
| 76 | Instantaneous Normal Mode Analysis of the Levitation Effect in Zeolites. Journal of Physical Chemistry B, 2000, 104, 709-715. | 2.6 | 16 |
| 77 | Isothermal-isobaric ensemble simulations of melting in quantum solids. Physical Review B, 1999, 59, 3590-3598. | 3.2 | 16 |
| 78 | Dynamics of Rare Gases in Zeolites: Instantaneous Normal Mode Analysis. Journal of Physical Chemistry B, 1999, 103, 2740-2748. | 2.6 | 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. | 3.0 | 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. | 2.1 | 30 |
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| 83 | Quantum Adsorbates:â€‰ Path Integral Monte Carlo Simulations of Helium in Silicalite. Journal of Physical Chemistry B, 1997, 101, 1878-1883. | 2.6 | 16 |
| 84 | Path integral simulations of atomic and molecular systems. International Reviews in Physical Chemistry, 1997, 16, 421-444. | 2.3 | 77 |
| 85 | Cluster analogs of binary isotopic mixtures: Path integral Monte Carlo simulations. Journal of Chemical Physics, 1996, 104, 7223-7232. | 3.0 | 11 |
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| 88 | Quantum delocalization and cluster melting. Journal of Chemical Physics, 1995, 103, 10663-10668. | 3.0 | 29 |
| 89 | Maximal Lyapunov exponent in small atomic clusters. Physical Review E, 1995, 51, 3376-3380. | 2.1 | 50 |
| 90 | 1/fSpectra in Finite Atomic Clusters. Physical Review Letters, 1995, 74, 4181-4184. | 7.8 | 23 |

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| 91 | Fourier path integral simulations ofpara-H2andortho-D2clusters. Molecular Physics, 1995, 84, 845-852. | 1.7 | 25 |
| 92 | Melting of neon clusters: Path integral Monte Carlo simulations. Journal of Chemical Physics, 1995, 102, 956-962. | 3.0 | 40 |
| 93 | STIMULATED EMISSION PUMPING AS A PROBE OF THE <font>OH</font> (X<sup>2</sup>Î) + <font>Ar</font> 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. | 3.0 | 52 |
| 95 | Particle exchange in the Fourier pathâ€integral Monte Carlo technique. Journal of Chemical Physics, 1993, 99, 8038-8043. | 3.0 | 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. | 2.6 | 63 |