Christopher J Mundy

List of Publications by Year
in descending order

120	8,285	50566	54771
papers	citations	48 h-index	88 g-index

122	122	122	7989
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Predictive Theoretical Framework for Dynamic Control of Bioinspired Hybrid Nanoparticle Self-Assembly. ACS Nano, 2022, 16, 1919-1928.	7.3	10
2	Hierarchical Self-Assembly Pathways of Peptoid Helices and Sheets. Biomacromolecules, 2022, 23, 992-1008.	2.6	19
3	Spiers Memorial Lecture: Assembly-based pathways of crystallization. Faraday Discussions, 2022, 235, 9-35.	1.6	10
4	Quantifying the Dynamics of Protein Self-Organization Using Deep Learning Analysis of Atomic Force Microscopy Data. Nano Letters, 2021, 21, 158-165.	4.5	17
5	Ion-dependent proteinâ€“surface interactions from intrinsic solvent response. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	10
6	Natural Charge-Transfer Analysis: Eliminating Spurious Charge-Transfer States in Time-Dependent Density Functional Theory via Diabatization, with Application to Projection-Based Embedding. Journal of Chemical Theory and Computation, 2021, 17, 4195-4210.	2.3	14
7	Toward a First-Principles Framework for Predicting Collective Properties of Electrolytes. Accounts of Chemical Research, 2021, 54, 2833-2843.	7.6	21
8	Visualizing Solution Structure at Solid-Liquid Interfaces using Three-Dimensional Fast Force Mapping. Journal of Visualized Experiments, 2021, , .	0.2	1
9	The Statistical Mechanics ofÂSolution-Phase Nucleation: CaCO$$_3$$ Revisited. Molecular Modeling and Simulation, 2021, , 101-122.	0.2	1
10	Moving beyond the Solvent-Tip Approximation to Determine Site-Specific Variations of Interfacial Water Structure through 3D Force Microscopy. Journal of Physical Chemistry C, 2021, 125, 1282-1291.	1.5	31
11	Probing the Thermodynamics and Kinetics of Ethylene Carbonate Reduction at the Electrode-Electrolyte Interface with Molecular Simulations. Journal of Chemical Physics, 2021, 155, 204703.	1.2	5
12	Quantifying the hydration structure of sodium and potassium ions: taking additional steps on Jacob's Ladder. Physical Chemistry Chemical Physics, 2020, 22, 10641-10652.	1.3	38
13	Solvent reaction coordinate for an SN2 reaction. Journal of Chemical Physics, 2020, 153, 024103.	1.2	11
14	MARTINI-Compatible Coarse-Grained Model for the Mesoscale Simulation of Peptoids. Journal of Physical Chemistry B, 2020, 124, 7745-7764.	1.2	28
15	Correlation function approach for diffusion in confined geometries. Physical Review E, 2020, 102, 022129.	0.8	6
16	Resolving Heterogeneous Dynamics of Excess Protons in Aqueous Solution with Rate Theory. Journal of Physical Chemistry B, 2020, 124, 5665-5675.	1.2	17
17	CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194103.	1.2	1,371
18	Nanometer-Scale Correlations in Aqueous Salt Solutions. Journal of Physical Chemistry Letters, 2020, 11, 2598-2604.	2.1	10

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19	Method for Accurately Predicting Solvation Structure. Journal of Chemical Theory and Computation, 2020, 16, 5401-5409.	2.3	12
20	Connecting energetics to dynamics in particle growth by oriented attachment using real-time observations. Nature Communications, 2020, 11, 1045.	5.8	74
21	Visualization of Aluminum Ions at the Mica Water Interface Links Hydrolysis State-to-Surface Potential and Particle Adhesion. Journal of the American Chemical Society, 2020, 142, 6093-6102.	6.6	24
22	Experimental and DFT Calculated IR Spectra of Guests in Zeolites: Acyclic Olefins and Hostâ€“Guest Interactions. Journal of Physical Chemistry C, 2020, 124, 10561-10572.	1.5	8
23	Molecular-level origin of the carboxylate head group response to divalent metal ion complexation at the airâ€“water interface. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 14874-14880.	3.3	37
24	The Diverse Nature of Ion Speciation at the Nanoscale Hydrophobic/Water Interface. Journal of Physical Chemistry B, 2019, 123, 2414-2423.	1.2	16
25	Direct Observation of the Orientational Anisotropy of Buried Hydroxyl Groups inside Muscovite Mica. Journal of the American Chemical Society, 2019, 141, 2135-2142.	6.6	23
26	Water Lone Pair Delocalization in Classical and Quantum Descriptions of the Hydration of Model Ions. Journal of Physical Chemistry B, 2018, 122, 3519-3527.	1.2	27
27	Peptoid Backbone Flexibility Dictates Its Interaction with Water and Surfaces: A Molecular Dynamics Investigation. Biomacromolecules, 2018, 19, 1006-1015.	2.6	28
28	Supersaturated calcium carbonate solutions are classical. Science Advances, 2018, 4, eaao6283.	4.7	116
29	On the relation between Marcus theory and ultrafast spectroscopy of solvation kinetics. Chemical Physics Letters, 2018, 692, 407-415.	1.2	10
30	Detecting the undetectable: The role of trace surfactant in the Jones-Ray effect. Journal of Chemical Physics, 2018, 149, 194702.	1.2	27
31	Diffusion Mechanisms of Radiolytic Species in Irradiated Al (Oxy-)Hydroxides. Journal of Physical Chemistry C, 2018, 122, 28990-28997.	1.5	12
32	Unraveling the spectral signatures of solvent ordering in K-edge XANES of aqueous Na+. Journal of Chemical Physics, 2018, 149, 124503.	1.2	12
33	Surface Chemistry Affects the Efficacy of the Hydration Force between Two ZnO(101Ì…0) Surfaces. Journal of Physical Chemistry C, 2018, 122, 12259-12266.	1.5	16
34	Understanding the scale of the single ion free energy: A critical test of the tetra-phenyl arsonium and tetra-phenyl borate assumption. Journal of Chemical Physics, 2018, 148, 222819.	1.2	18
35	Revisiting the hydration structure of aqueous Na+. Journal of Chemical Physics, 2017, 146, 084504.	1.2	90
36	Tuning crystallization pathways through sequence engineering of biomimetic polymers. Nature Materials, 2017, 16, 767-774.	13.3	116

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37	Electrostatic solvation free energies of charged hard spheres using molecular dynamics with density functional theory interactions. Journal of Chemical Physics, 2017, 147, 161716.	1.2	42
38	Marcus Theory of Ion-Pairing. Journal of Chemical Theory and Computation, 2017, 13, 3470-3477.	2.3	53
39	Quantifying the Molecular-Scale Aqueous Response to the Mica Surface. Journal of Physical Chemistry C, 2017, 121, 18496-18504.	1.5	19
40	Real single ion solvation free energies with quantum mechanical simulation. Chemical Science, 2017, 8, 6131-6140.	3.7	63
41	Trends in micaâ€“mica adhesion reflect the influence of molecular details on long-range dispersion forces underlying aggregation and coalignment. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 7537-7542.	3.3	56
42	Mass density fluctuations in quantum and classical descriptions of liquid water. Journal of Chemical Physics, 2017, 146, 244501.	1.2	44
43	The structure of liquid water up to 360 MPa from x-ray diffraction measurements using a high Q-range and from molecular simulation. Journal of Chemical Physics, 2016, 144, 134504.	1.2	38
44	Reaction Rate Theory in Coordination Number Space: An Application to Ion Solvation. Journal of Physical Chemistry C, 2016, 120, 7597-7605.	1.5	36
45	Smoothed dissipative particle dynamics model for mesoscopic multiphase flows in the presence of thermal fluctuations. Physical Review E, 2016, 94, 023304.	0.8	11
46	Ions interacting in solution: Moving from intrinsic to collective properties. Current Opinion in Colloid and Interface Science, 2016, 23, 58-65.	3.4	29
47	Divalent Ion Parameterization Strongly Affects Conformation and Interactions of an Anionic Biomimetic Polymer. Journal of Physical Chemistry B, 2016, 120, 2198-2208.	1.2	18
48	Dependence of the Rate of LiF Ion-Pairing on the Description of Molecular Interaction. Journal of Physical Chemistry B, 2016, 120, 1749-1758.	1.2	13
49	Local Aqueous Solvation Structure Around Ca²⁺ During Ca²⁺Â·Â·Â·Cl^{â€“} Pair Formation. Journal of Physical Chemistry B, 2016, 120, 1885-1893.	1.2	40
50	The Role of Solvent Heterogeneity in Determining the Dispersion Interaction between Nanoassemblies. Journal of Physical Chemistry B, 2015, 119, 5873-5881.	1.2	26
51	Modeling nanoscale hydrodynamics by smoothed dissipative particle dynamics. Journal of Chemical Physics, 2015, 142, 194504.	1.2	17
52	Aqueous Cation-Amide Binding: Free Energies and IR Spectral Signatures by Ab Initio Molecular Dynamics. Journal of Physical Chemistry Letters, 2014, 5, 2235-2240.	2.1	37
53	Investigation of Interfacial and Bulk Dissociation of HBr, HCl, and HNO₃ Using Density Functional Theory-Based Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2014, 118, 29412-29420.	1.5	40
54	The Role of Broken Symmetry in Solvation of a Spherical Cavity in Classical and Quantum Water Models. Journal of Physical Chemistry Letters, 2014, 5, 2767-2774.	2.1	71

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55	Toward a Unified Picture of the Water Self-Ions at the Airâ€“Water Interface: A Density Functional Theory Perspective. Journal of Physical Chemistry B, 2014, 118, 8364-8372.	1.2	90
56	Persistent Ion Pairing in Aqueous Hydrochloric Acid. Journal of Physical Chemistry B, 2014, 118, 7211-7220.	1.2	53
57	Calculation of the Gibbs free energy of solvation and dissociation of HCl in water via Monte Carlo simulations and continuum solvation models. Physical Chemistry Chemical Physics, 2013, 15, 13578.	1.3	39
58	Ab Initio Molecular Dynamics Simulation of Proton Hopping in a Model Polymer Membrane. Journal of Physical Chemistry B, 2013, 117, 16522-16529.	1.2	50
59	Thermodynamics of iodide adsorption at the instantaneous air-water interface. Journal of Chemical Physics, 2013, 138, 114709.	1.2	48
60	An ab initio approach to understanding the specific ion effect. Faraday Discussions, 2013, 160, 89-101.	1.6	49
61	Simulation and Theory of Ions at Atmospherically Relevant Aqueous Liquid-Air Interfaces. Annual Review of Physical Chemistry, 2013, 64, 339-359.	4.8	151
62	Implementing the Data Center Energy Productivity Metric in a High-Performance Computing Data Center. , 2013, , 93-116.		1
63	Implementing the data center energy productivity metric. ACM Journal on Emerging Technologies in Computing Systems, 2012, 8, 1-22.	1.8	7
64	Understanding Vibrational Anharmonicity and Phonon Dispersion in Solid Ammonia Borane. Journal of Physical Chemistry C, 2012, 116, 5926-5931.	1.5	10
65	Polarization- and Azimuth-Resolved Infrared Spectroscopy of Water on TiO₂(110): Anisotropy and the Hydrogen-Bonding Network. Journal of Physical Chemistry Letters, 2012, 3, 778-784.	2.1	91
66	Electrochemical Surface Potential Due to Classical Point Charge Models Drives Anion Adsorption to the Airâ€“Water Interface. Journal of Physical Chemistry Letters, 2012, 3, 1565-1570.	2.1	67
67	Toward an Understanding of the Specific Ion Effect Using Density Functional Theory. Journal of Physical Chemistry Letters, 2011, 2, 1088-1093.	2.1	114
68	Understanding the Surface Potential of Water. Journal of Physical Chemistry B, 2011, 115, 4369-4377.	1.2	157
69	Vaporâ€“Liquid Coexistence Curves for Methanol and Methane Using Dispersion-Corrected Density Functional Theory. Journal of Physical Chemistry B, 2011, 115, 11688-11692.	1.2	38
70	Is Iodate a Strongly Hydrated Cation?. Journal of Physical Chemistry Letters, 2011, 2, 2650-2654.	2.1	68
71	Dissociation of Strong Acid Revisited: X-ray Photoelectron Spectroscopy and Molecular Dynamics Simulations of HNO₃ in Water. Journal of Physical Chemistry B, 2011, 115, 9445-9451.	1.2	46
72	Does Nitric Acid Dissociate at the Aqueous Solution Surface?. Journal of Physical Chemistry C, 2011, 115, 21183-21190.	1.5	73

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73	Semiempirical Self-Consistent Polarization Description of Bulk Water, the Liquidâ^'Vapor Interface, and Cubic Ice. Journal of Physical Chemistry A, 2011, 115, 6046-6053.	1.1	22
74	Re-examining the properties of the aqueous vaporâ€"liquid interface using dispersion corrected density functional theory. Journal of Chemical Physics, 2011, 135, 124712.	1.2	82
75	Improving the density functional theory description of water with self-consistent polarization. Journal of Chemical Physics, 2010, 132, 164102.	1.2	30
76	Interpreting Vibrational Sum-Frequency Spectra of Sulfur Dioxide at the Air/Water Interface: A Comprehensive Molecular Dynamics Study. Journal of Physical Chemistry B, 2010, 114, 7245-7249.	1.2	27
77	Probing the Hydration Structure of Polarizable Halides: A Multiedge XAFS and Molecular Dynamics Study of the Iodide Anion. Journal of Physical Chemistry B, 2010, 114, 12926-12937.	1.2	78
78	First principles Monte Carlo simulations of aggregation in the vapor phase of hydrogen fluoride. Physical Chemistry Chemical Physics, 2010, 12, 7678.	1.3	18
79	Ab initio simulation of the equation of state and kinetics of shocked water. Journal of Chemical Physics, 2009, 130, 124517.	1.2	91
80	Vaporâ€"liquid phase equilibria of water modelled by a Kimâ€"Gordon potential. Chemical Physics Letters, 2009, 479, 60-64.	1.2	2
81	Hydroxide anion at the airâ€"water interface. Chemical Physics Letters, 2009, 481, 2-8.	1.2	118
82	Isobaricâ^'Isothermal Molecular Dynamics Simulations Utilizing Density Functional Theory: An Assessment of the Structure and Density of Water at Near-Ambient Conditions. Journal of Physical Chemistry B, 2009, 113, 11959-11964.	1.2	327
83	Self-Consistent Polarization Density Functional Theory: Application to Argon. Journal of Physical Chemistry A, 2009, 113, 2075-2085.	1.1	19
84	No Confinement Needed: Observation of a Metastable Hydrophobic Wetting Two-Layer Ice on Graphene. Journal of the American Chemical Society, 2009, 131, 12838-12844.	6.6	186
85	Neutron Powder Diffraction and Molecular Simulation Study of the Structural Evolution of Ammonia Borane from 15 to 340 K. Journal of Physical Chemistry A, 2009, 113, 5723-5735.	1.1	56
86	Spectral Signatures of the Pentagonal Water Cluster in Bacteriorhodopsin. ChemPhysChem, 2008, 9, 2703-2707.	1.0	32
87	Electronic Effects on the Surface Potential at the Vaporâ^'Liquid Interface of Water. Journal of the American Chemical Society, 2008, 130, 16556-16561.	6.6	134
88	Ultrafast transformation of graphite to diamond: An ab initio study of graphite under shock compression. Journal of Chemical Physics, 2008, 128, 184701.	1.2	84
89	Structure of the Methanol Liquidâ^'Vapor Interface: A Comprehensive Particle-Based Simulation Study. Journal of Physical Chemistry C, 2008, 112, 15412-15418.	1.5	23
90	AB INITIO MOLECULAR DYNAMICS SIMULATIONS OF WATER UNDER STATIC AND SHOCK COMPRESSED CONDITIONS. AIP Conference Proceedings, 2008, , .	0.3	2

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91	A molecular approach to understanding complex systems: computational statistical mechanics using state-of-the-art algorithms on terascale computational platforms. Journal of Physics: Conference Series, 2008, 125, 012014.	0.3	1
92	QM/MM Metadynamics Study of the Direct Decarboxylation Mechanism for Orotidine-5â€˜-monophosphate Decarboxylase Using Two Different QM Regions:â€‰ Acceleration Too Small To Explain Rate of Enzyme Catalysis. Journal of Physical Chemistry B, 2007, 111, 12573-12581.	1.2	53
93	Spatial correlation of dipole fluctuations in liquid water. Molecular Physics, 2007, 105, 1411-1417.	0.8	25
94	The Effect of Polarizability for Understanding the Molecular Structure of Aqueous Interfaces. Journal of Chemical Theory and Computation, 2007, 3, 2002-2010.	2.3	110
95	Acid/base equilibria in clusters and their role in proton exchange membranes: computational insight. Physical Chemistry Chemical Physics, 2007, 9, 5752.	1.3	48
96	Time-Dependent Properties of Liquid Water:â€‰ A Comparison of Carâ€'Parrinello and Bornâ€'Oppenheimer Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2006, 2, 1274-1281.	2.3	77
97	Molecular Dynamics Simulation of Liquid Water:Â Hybrid Density Functionalsâ€. Journal of Physical Chemistry B, 2006, 110, 3685-3691.	1.2	242
98	Simulating Fluid-Phase Equilibria of Water from First Principlesâ€. Journal of Physical Chemistry A, 2006, 110, 640-646.	1.1	128
99	First-Principles Approaches to the Structure and Reactivity of Atmospherically Relevant Aqueous Interfaces. Chemical Reviews, 2006, 106, 1282-1304.	23.0	71
100	Structure and Dynamics of the Aqueous Liquidâ€'Vapor Interface:Â A Comprehensive Particle-Based Simulation StudyâŠ¥. Journal of Physical Chemistry B, 2006, 110, 3738-3746.	1.2	115
101	Vaporâ€“liquid equilibria of water from first principles: comparison of density functionals and basis sets. Molecular Physics, 2006, 104, 3619-3626.	0.8	79
102	Chemistry of H2O and HF under Extreme Conditions. AIP Conference Proceedings, 2006, , .	0.3	0
103	Isobaric-Isothermal Monte Carlo Simulations from First Principles: Application to Liquid Water at Ambient Conditions. ChemPhysChem, 2005, 6, 1894-1901.	1.0	99
104	Toward a Monte Carlo program for simulating vaporâ€“liquid phase equilibria from first principles. Computer Physics Communications, 2005, 169, 289-294.	3.0	29
105	Dynamic Ionization of Water under Extreme Conditions. Physical Review Letters, 2005, 94, 125508.	2.9	212
106	Structure of dense hydrogen fluoride gas from neutron diffraction and molecular dynamics simulations. Journal of Chemical Physics, 2005, 122, 154511.	1.2	13
107	Bonding in the Superionic Phase of Water. Physical Review Letters, 2005, 94, 217801.	2.9	99
108	A density-functional approach to polarizable models: A Kim-Gordon response density interaction potential for molecular simulations. Journal of Chemical Physics, 2005, 123, 074108.	1.2	14

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109	HYDROPHOBIC HYDRATION FROM CARâ€“PARRINELLO SIMULATIONS. International Journal of Modern Physics B, 2004, 18, 1951-1962.	1.0	29
110	Liquid Water from First Principles:Â Investigation of Different Sampling Approaches. Journal of Physical Chemistry B, 2004, 108, 12990-12998.	1.2	327
111	An ab Initio Molecular Dynamics Study of the Aqueous Liquid-Vapor Interface. Science, 2004, 303, 658-660.	6.0	325
112	On the Mechanisms of OH Radical Induced DNA-Base Damage:Â A Comparative Quantum Chemical and Carâ˜Parrinello Molecular Dynamics Studyâ€. Journal of Physical Chemistry A, 2004, 108, 2922-2929.	1.1	54
113	Classical polarizable force fields parametrized from ab initio calculations. Journal of Chemical Physics, 2002, 117, 1416-1433.	1.2	61
114	Irradiated Guanine:â€‰ A Car-Parrinello Molecular Dynamics Study of Dehydrogenation in the Presence of an OH Radical. Journal of Physical Chemistry A, 2002, 106, 10063-10071.	1.1	66
115	Formation of a Reactive Intermediate in Molecular Beam Chemistry of Sodium and Water. Journal of Physical Chemistry A, 2001, 105, 8423-8427.	1.1	28
116	General and efficient algorithms for obtaining maximally localized Wannier functions. Physical Review B, 2000, 61, 10040-10048.	1.1	272
117	Microsolvation and Chemical Reactivity of Sodium and Water Clusters. Journal of the American Chemical Society, 2000, 122, 4837-4838.	6.6	66
118	On the classical statistical mechanics of non-Hamiltonian systems. Europhysics Letters, 1999, 45, 149-155.	0.7	138
119	Viscosity of selfâ€assembled fluids. Journal of Chemical Physics, 1992, 97, 7695-7698.	1.2	10
120	Renormalization of a Landau-Ginzburg-Wilson theory of microemulsion. Physical Review A, 1992, 45, 7309-7319.	1.0	30