Christopher D Daub

List of Publications by Year
in descending order

33	932	567281 15	434195 31
papers	citations	h-index	g-index

34	34	34	877
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Effect of Field Direction on Electrowetting in a Nanopore. Journal of the American Chemical Society, 2007, 129, 2504-2510.	13.7	175
2	Electrowetting at the Nanoscale. Journal of Physical Chemistry C, 2007, 111, 505-509.	3.1	137
3	The influence of molecular-scale roughness on the surface spreading of an aqueous nanodrop. Faraday Discussions, 2010, 146, 67.	3.2	76
4	Electric Control of Wetting by Salty Nanodrops: Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2011, 115, 22393-22399.	3.1	59
5	Water-mediated ordering of nanoparticles in an electric field. Faraday Discussions, 2009, 141, 55-66.	3.2	54
6	Monte Carlo simulations of the adsorption of CO2 on the MgO(100) surface. Journal of Chemical Physics, 2006, 124, 114706.	3.0	52
7	The role of electron correlation on calculated XH-stretching vibrational band intensities. Molecular Physics, 1997, 90, 201-213.	1.7	49
8	Field-exposed water in a nanopore: liquid or vapour?. Physical Chemistry Chemical Physics, 2008, 10, 6807.	2.8	44
9	How Are Completely Desolvated Ions Produced in Electrospray Ionization: Insights from Molecular Dynamics Simulations. Analytical Chemistry, 2011, 83, 8372-8376.	6.5	43
10	Microscopic Dynamics of the Orientation of a Hydrated Nanoparticle in an Electric Field. Physical Review Letters, 2009, 103, 207801.	7.8	32
11	Nanoscale Wetting Under Electric Field from Molecular Simulations. Topics in Current Chemistry, 2011, 307, 155-179.	4.0	27
12	Structure of Aqueous Solutions of Monosodium Glutamate. Journal of Physical Chemistry B, 2009, 113, 7687-7700.	2.6	21
13	Electrokinetic flow of an aqueous electrolyte in amorphous silica nanotubes. Physical Chemistry Chemical Physics, 2018, 20, 27838-27848.	2.8	18
14	Liquidâ€“vapor criticality in a fluid of charged hard dumbbells. Journal of Chemical Physics, 2003, 119, 7952-7956.	3.0	17
15	Modelling and calculation of dipole moment functions for XH bonds. Canadian Journal of Chemistry, 1999, 77, 1775-1781.	1.1	15
16	Fragmentation inside proton-transfer-reaction-based mass spectrometers limits the detection of ROOR and ROOH peroxides. Atmospheric Measurement Techniques, 2022, 15, 1811-1827.	3.1	14
17	Lithium Ionâ€“Water Clusters in Strong Electric Fields: A Quantum Chemical Study. Journal of Physical Chemistry A, 2015, 119, 4983-4992.	2.5	12
18	Thermo-molecular orientation effects in fluids of dipolar dumbbells. Physical Chemistry Chemical Physics, 2014, 16, 22097-22106.	2.8	11

#	Article	IF	Citations
19	Local Field Factors and Dielectric Properties of Liquid Benzene. Journal of Physical Chemistry B, 2015, 119, 11839-11845.	2.6	9
20	Note: How does the treatment of electrostatic interactions influence the magnitude of thermal polarization of water? The SPC/E model. Journal of Chemical Physics, 2015, 143, 036101.	3.0	8
21	Molecular alignment in molecular fluids induced by coupling between density and thermal gradients. Physical Chemistry Chemical Physics, 2016, 18, 12213-12220.	2.8	7
22	Ab Initio Molecular Dynamics Simulations of the Influence of Lithium Bromide Salt on the Deprotonation of Formic Acid in Aqueous Solution. Journal of Physical Chemistry B, 2019, 123, 6823-6829.	2.6	7
23	The constant-volume heat capacity of near-critical fluids with long-range interactions: A discussion of different Monte Carlo estimates. Journal of Chemical Physics, 2003, 118, 4164-4168.	3.0	6
24	Modelling and calculation of dipole moment functions for XH bonds. Canadian Journal of Chemistry, 1999, 77, 1775-1781.	1.1	6
25	Energy transfer, pre-reactive complex formation and recombination reactions during the collision of peroxy radicals. Physical Chemistry Chemical Physics, 2022, 24, 10033-10043.	2.8	6
26	Molecular Dynamics Simulations to Examine Structure, Energetics, and Evaporation/Condensation Dynamics in Small Charged Clusters of Water or Methanol Containing a Single Monatomic Ion. Journal of Physical Chemistry A, 2012, 116, 10488-10495.	2.5	5
27	Chemistrees: Data-Driven Identification of Reaction Pathways via Machine Learning. Journal of Chemical Theory and Computation, 2021, 17, 6193-6202.	5.3	5
28	Path sampling for atmospheric reactions: formic acid catalysed conversion of SO₃ + H₂O to H₂SO₄. PeerJ Physical Chemistry, 0, 2, e7.	0.0	5
29	Constant-volume heat capacity in a near-critical fluid from Monte Carlo simulations. Journal of Chemical Physics, 2004, 121, 8956-8959.	3.0	4
30	Ab Initio Molecular Dynamics Simulations of the Influence of Lithium Bromide on the Structure of the Aqueous Solutionâ€“Air Interface. Journal of Physical Chemistry B, 2019, 123, 729-737.	2.6	4
31	Polarisation of polar dumbbell fluids in thermal gradients: the importance of the treatment of electrostatic interactions. Molecular Physics, 2016, 114, 3249-3254.	1.7	3
32	Manipulation of Liquid Crystals by an Orienting Force in MD Simulations. Ferroelectrics, 2012, 431, 99-107.	0.6	1
33	Atomistic simulations of the local electric field in dielectric liquids. , 2014, , .		0