Thomas F Headen

List of Publications by Year
in descending order

35 papers	1,622 citations	394421 19 h-index	345221 36 g-index
37 all docs	37 docs citations	37 times ranked	1757 citing authors

#	Article	IF	Citations
1	A revised mechanistic model for sodium insertion in hard carbons. Energy and Environmental Science, 2020, 13, 3469-3479.	30.8	195
2	Evidence for Asphaltene Nanoaggregation in Toluene and Heptane from Molecular Dynamics Simulations. Energy & Fuels, 2009, 23, 1220-1229.	5.1	193
3	Structure of Ï€â^'Ï€ Interactions in Aromatic Liquids. Journal of the American Chemical Society, 2010, 132, 5735-5742.	13.7	177
4	Simulation of Asphaltene Aggregation through Molecular Dynamics: Insights and Limitations. Energy & Fuels, 2017, 31, 1108-1125.	5.1	170
5	Quantitative Molecular Representation of Asphaltenes and Molecular Dynamics Simulation of Their Aggregation. Energy & Fuels, 2009, 23, 1209-1219.	5.1	167
6	Molecular Dynamics Simulations of Asphaltene Aggregation in Supercritical Carbon Dioxide with and without Limonene. Energy & Fuels, 2011, 25, 503-508.	5.1	77
7	Liquid phase blending of metal-organic frameworks. Nature Communications, 2018, 9, 2135.	12.8	69
8	Small Angle Neutron Scattering (SANS and V-SANS) Study of Asphaltene Aggregates in Crude Oil. Langmuir, 2009, 25, 422-428.	3.5	67
9	Sodium Storage Mechanism Investigations through Structural Changes in Hard Carbons. ACS Applied Energy Materials, 2020, 3, 9918-9927.	5.1	56
10	Multi-scale Simulation and Experimental Studies of Asphaltene Aggregation and Deposition in Capillary Flow. Energy & Fuels, 2010, 24, 2361-2368.	5.1	54
11	Potential of Mean Force Calculation from Molecular Dynamics Simulation of Asphaltene Molecules on a Calcite Surface. Energy & Fuels, 2011, 25, 499-502.	5.1	42
12	Catalogue of Plausible Molecular Models for the Molecular Dynamics of Asphaltenes and Resins Obtained from Quantitative Molecular Representation. Energy & Fuels, 2019, 33, 9779-9795.	5.1	34
13	Adsorption of asphaltenes on the calcite (10.4) surface by first-principles calculations. RSC Advances, 2016, 6, 95328-95336.	3.6	31
14	Ammonia boraneâ€“polyethylene oxide composite materials for solid hydrogen storage. Journal of Materials Chemistry A, 2015, 3, 3683-3691.	10.3	28
15	Local Structure and Polar Order in Liquid N-Methyl-2-pyrrolidone (NMP). Journal of Physical Chemistry B, 2018, 122, 8963-8971.	2.6	27
16	Predicting Asphaltene Aggregate Structure from Molecular Dynamics Simulation: Comparison to Neutron Total Scattering Data. Energy & Fuels, 2019, 33, 3787-3795.	5.1	27
17	Multi-scale simulation of asphaltene aggregation and deposition in capillary flow. Faraday Discussions, 2010, 144, 271-284.	3.2	26
18	Micrometer-sized Water Ice Particles for Planetary Science Experiments: Influence of Surface Structure on Collisional Properties. Astrophysical Journal, 2017, 848, 96.	4.5	25

#	Article	IF	Citations
19	The structures of liquid pyridine and naphthalene: the effects of heteroatoms and core size on aromatic interactions. Physical Chemistry Chemical Physics, 2018, 20, 2704-2715.	2.8	20
20	The liquid structure of the solvents dimethylformamide (DMF) and dimethylacetamide (DMA). Molecular Physics, 2019, 117, 3353-3363.	1.7	19
21	Elucidation of the Solid Electrolyte Interphase Formation Mechanism in Microâ€Mesoporous Hardâ€Carbon Anodes. Advanced Materials Interfaces, 2022, 9, 2101267.	3.7	18
22	Superalkaliâ€“Alkalide Interactions and Ion Pairing in Low-Polarity Solvents. Journal of the American Chemical Society, 2021, 143, 3934-3943.	13.7	17
23	Filtration of deformable emulsion droplets. Journal of Colloid and Interface Science, 2006, 304, 562-565.	9.4	16
24	Temperature dependent structural changes in liquid benzene studied using neutron diffraction. Molecular Physics, 2019, 117, 3329-3336.	1.7	13
25	Dihydrogen vs. hydrogen bonding in the solvation of ammonia borane by tetrahydrofuran and liquid ammonia. Physical Chemistry Chemical Physics, 2018, 20, 12200-12209.	2.8	11
26	Exploring Methane Behavior in Marcellus Shale Micropores via Contrast Matching Neutron Scattering. Energy & Fuels, 2020, 34, 10926-10932.	5.1	7
27	Bulk and Confined Benzene-Cyclohexane Mixtures Studied by an Integrated Total Neutron Scattering and NMR Method. Topics in Catalysis, 2021, 64, 722-734.	2.8	6
28	Solvent Effects on the Structure of Petroleum Asphaltenes. Energy & Fuels, 2021, 35, 13743-13755.	5.1	6
29	Impacts of Mineralogical Variation on CO₂ Behavior in Small Pores from Producing Intervals of the Marcellus Shale: Results from Neutron Scattering. Energy & Fuels, 2020, 34, 2765-2771.	5.1	5
30	Neutron studies of Na-ion battery materials. JPhys Materials, 2021, 4, 042008.	4.2	5
31	Neutron total scattering investigation on the dissolution mechanism of trehalose in NaOH/urea aqueous solution. Structural Dynamics, 2021, 8, 014901.	2.3	5
32	Subtle changes in hydrogen bond orientation result in glassification of carbon capture solvents. Physical Chemistry Chemical Physics, 2020, 22, 19009-19021.	2.8	3
33	Toward unveiling structure and property relationships from ionic ordering in Li/S battery electrolytes: Neutron total scattering and molecular dynamics simulations. Energy Storage Materials, 2022, 52, 85-93.	18.0	2
34	Intermediate Range Order in Metalâ€“Ammonia Solutions: Pure and Na-Doped Ca-NH₃. Journal of Physical Chemistry B, 2021, 125, 7456-7461.	2.6	1
35	Atomic structure of the continuous random network of amorphous C[(C6H4)2]2 PAF-1. Cell Reports Physical Science, 2022, , 100899.	5.6	0