

# Thomas F Headen

## List of Publications by Year in descending order

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35  
papers

1,622  
citations

394421

19  
h-index

345221

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g-index

37  
all docs

37  
docs citations

37  
times ranked

1757  
citing authors

#	ARTICLE	IF	CITATIONS
1	Elucidation of the Solid Electrolyte Interphase Formation Mechanism in Micro-Mesoporous Hard-Carbon Anodes. <i>Advanced Materials Interfaces</i> , 2022, 9, 2101267.	3.7	18
2	Atomic structure of the continuous random network of amorphous C[(C <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> ] <sub>2</sub> PAF-1. <i>Cell Reports Physical Science</i> , 2022, , 100899.	5.6	0
3	Toward unveiling structure and property relationships from ionic ordering in Li/S battery electrolytes: Neutron total scattering and molecular dynamics simulations. <i>Energy Storage Materials</i> , 2022, 52, 85-93.	18.0	2
4	Superalkali-Alkalide Interactions and Ion Pairing in Low-Polarity Solvents. <i>Journal of the American Chemical Society</i> , 2021, 143, 3934-3943.	13.7	17
5	Bulk and Confined Benzene-Cyclohexane Mixtures Studied by an Integrated Total Neutron Scattering and NMR Method. <i>Topics in Catalysis</i> , 2021, 64, 722-734.	2.8	6
6	Intermediate Range Order in Metal-Ammonia Solutions: Pure and Na-Doped Ca-NH <sub>3</sub> . <i>Journal of Physical Chemistry B</i> , 2021, 125, 7456-7461.	2.6	1
7	Solvent Effects on the Structure of Petroleum Asphaltenes. <i>Energy &amp; Fuels</i> , 2021, 35, 13743-13755.	5.1	6
8	Neutron studies of Na-ion battery materials. <i>JPhys Materials</i> , 2021, 4, 042008.	4.2	5
9	Neutron total scattering investigation on the dissolution mechanism of trehalose in NaOH/urea aqueous solution. <i>Structural Dynamics</i> , 2021, 8, 014901.	2.3	5
10	A revised mechanistic model for sodium insertion in hard carbons. <i>Energy and Environmental Science</i> , 2020, 13, 3469-3479.	30.8	195
11	Exploring Methane Behavior in Marcellus Shale Micropores via Contrast Matching Neutron Scattering. <i>Energy &amp; Fuels</i> , 2020, 34, 10926-10932.	5.1	7
12	Sodium Storage Mechanism Investigations through Structural Changes in Hard Carbons. <i>ACS Applied Energy Materials</i> , 2020, 3, 9918-9927.	5.1	56
13	Subtle changes in hydrogen bond orientation result in glassification of carbon capture solvents. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 19009-19021.	2.8	3
14	Impacts of Mineralogical Variation on CO <sub>2</sub> Behavior in Small Pores from Producing Intervals of the Marcellus Shale: Results from Neutron Scattering. <i>Energy &amp; Fuels</i> , 2020, 34, 2765-2771.	5.1	5
15	The liquid structure of the solvents dimethylformamide (DMF) and dimethylacetamide (DMA). <i>Molecular Physics</i> , 2019, 117, 3353-3363.	1.7	19
16	Temperature dependent structural changes in liquid benzene studied using neutron diffraction. <i>Molecular Physics</i> , 2019, 117, 3329-3336.	1.7	13
17	Catalogue of Plausible Molecular Models for the Molecular Dynamics of Asphaltenes and Resins Obtained from Quantitative Molecular Representation. <i>Energy &amp; Fuels</i> , 2019, 33, 9779-9795.	5.1	34
18	Predicting Asphaltene Aggregate Structure from Molecular Dynamics Simulation: Comparison to Neutron Total Scattering Data. <i>Energy &amp; Fuels</i> , 2019, 33, 3787-3795.	5.1	27

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19	Dihydrogen vs. hydrogen bonding in the solvation of ammonia borane by tetrahydrofuran and liquid ammonia. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 12200-12209.	2.8	11
20	The structures of liquid pyridine and naphthalene: the effects of heteroatoms and core size on aromatic interactions. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2704-2715.	2.8	20
21	Local Structure and Polar Order in Liquid <i>N</i> -Methyl-2-pyrrolidone (NMP). <i>Journal of Physical Chemistry B</i> , 2018, 122, 8963-8971.	2.6	27
22	Liquid phase blending of metal-organic frameworks. <i>Nature Communications</i> , 2018, 9, 2135.	12.8	69
23	Simulation of Asphaltene Aggregation through Molecular Dynamics: Insights and Limitations. <i>Energy &amp; Fuels</i> , 2017, 31, 1108-1125.	5.1	170
24	Micrometer-sized Water Ice Particles for Planetary Science Experiments: Influence of Surface Structure on Collisional Properties. <i>Astrophysical Journal</i> , 2017, 848, 96.	4.5	25
25	Adsorption of asphaltenes on the calcite (10.4) surface by first-principles calculations. <i>RSC Advances</i> , 2016, 6, 95328-95336.	3.6	31
26	Ammonia borane-polyethylene oxide composite materials for solid hydrogen storage. <i>Journal of Materials Chemistry A</i> , 2015, 3, 3683-3691.	10.3	28
27	Potential of Mean Force Calculation from Molecular Dynamics Simulation of Asphaltene Molecules on a Calcite Surface. <i>Energy &amp; Fuels</i> , 2011, 25, 499-502.	5.1	42
28	Molecular Dynamics Simulations of Asphaltene Aggregation in Supercritical Carbon Dioxide with and without Limonene. <i>Energy &amp; Fuels</i> , 2011, 25, 503-508.	5.1	77
29	Structure of $\pi$ - $\pi$ Interactions in Aromatic Liquids. <i>Journal of the American Chemical Society</i> , 2010, 132, 5735-5742.	13.7	177
30	Multi-scale simulation of asphaltene aggregation and deposition in capillary flow. <i>Faraday Discussions</i> , 2010, 144, 271-284.	3.2	26
31	Multi-scale Simulation and Experimental Studies of Asphaltene Aggregation and Deposition in Capillary Flow. <i>Energy &amp; Fuels</i> , 2010, 24, 2361-2368.	5.1	54
32	Quantitative Molecular Representation of Asphaltenes and Molecular Dynamics Simulation of Their Aggregation. <i>Energy &amp; Fuels</i> , 2009, 23, 1209-1219.	5.1	167
33	Small Angle Neutron Scattering (SANS and V-SANS) Study of Asphaltene Aggregates in Crude Oil. <i>Langmuir</i> , 2009, 25, 422-428.	3.5	67
34	Evidence for Asphaltene Nanoaggregation in Toluene and Heptane from Molecular Dynamics Simulations. <i>Energy &amp; Fuels</i> , 2009, 23, 1220-1229.	5.1	193
35	Filtration of deformable emulsion droplets. <i>Journal of Colloid and Interface Science</i> , 2006, 304, 562-565.	9.4	16