David S Sholl

List of Publications by Citations

240 papers	16,759 citations	70 h-index	122 g-index
249 ext. papers	19,279 ext. citations	7.2 avg, IF	7.47 L-index

#	Paper	IF	Citations
240	Seven chemical separations to change the world. *Nature*, **2016**, 532, 435-7	50.4	1625
239	Can metal-organic framework materials play a useful role in large-scale carbon dioxide separations?. *ChemSusChem*, **2010**, 3, 879-91	8.3	518
238	**2009**,		395
237	Chiral selection on inorganic crystalline surfaces. *Nature Materials*, **2003**, 2, 367-74	27	389
236	Computation-Ready, Experimental Metal□Organic Frameworks: A Tool To Enable High-Throughput Screening of Nanoporous Crystals. *Chemistry of Materials*, **2014**, 26, 6185-6192	9.6	387
235	Self-diffusion and transport diffusion of light gases in metal-organic framework materials assessed using molecular dynamics simulations. *Journal of Physical Chemistry B*, **2005**, 109, 15760-8	3.4	374
234	Nanoscale design to enable the revolution in renewable energy. *Energy and Environmental Science*, **2009**, 2, 559	35.4	311
233	Chemically Meaningful Atomic Charges That Reproduce the Electrostatic Potential in Periodic and Nonperiodic Materials. *Journal of Chemical Theory and Computation*, **2010**, 6, 2455-68	6.4	282
232	Progress, Opportunities, and Challenges for Applying Atomically Detailed Modeling to Molecular Adsorption and Transport in Metal□Organic Framework Materials. *Industrial & Engineering Chemistry Research*, **2009**, 48, 2355-2371	3.9	270
231	The materials genome in action: identifying the performance limits for methane storage. *Energy and Environmental Science*, **2015**, 8, 1190-1199	35.4	263
230	Ultem□ /ZIF-8 mixed matrix hollow fiber membranes for CO2/N2 separations. *Journal of Membrane Science*, **2012**, 401-402, 76-82	9.6	253
229	Exploring the Framework Hydrophobicity and Flexibility of ZIF-8: From Biofuel Recovery to Hydrocarbon Separations. *Journal of Physical Chemistry Letters*, **2013**, 4, 3618-3622	6.4	242
228	Efficient calculation of diffusion limitations in metal organic framework materials: a tool for identifying materials for kinetic separations. *Journal of the American Chemical Society*, **2010**, 132, 7528-39	16.4	239
227	From water to organics in membrane separations. *Nature Materials*, **2017**, 16, 276-279	27	235
226	Defects in Metal-Organic Frameworks: Challenge or Opportunity?. *Journal of Physical Chemistry Letters*, **2015**, 6, 3437-44	6.4	230
225	Modification of the Mg/DOBDC MOF with Amines to Enhance CO2 Adsorption from Ultradilute Gases. *Journal of Physical Chemistry Letters*, **2012**, 3, 1136-41	6.4	221
224	Predicting multicomponent adsorption: 50 years of the ideal adsorbed solution theory. *AICHE Journal*, **2015**, 61, 2757-2762	3.6	219

223	Improved Atoms-in-Molecule Charge Partitioning Functional for Simultaneously Reproducing the Electrostatic Potential and Chemical States in Periodic and Nonperiodic Materials. *Journal of Chemical Theory and Computation*, **2012**, 8, 2844-67	6.4	210
222	Transport Diffusivities of CH4, CF4, He, Ne, Ar, Xe, and SF6 in Silicalite from Atomistic Simulations. *Journal of Physical Chemistry B*, **2002**, 106, 5058-5067	3.4	193
221	Naturally Chiral Metal Surfaces as Enantiospecific Adsorbents. *Journal of Physical Chemistry B*, **2001**, 105, 4771-4782	3.4	184
220	Advances, Updates, and Analytics for the Computation-Ready, Experimental Metal□Organic Framework Database: CoRE MOF 2019. *Journal of Chemical & Engineering Data*, **2019**, 64, 5985-5998	2.8	183
219	Materials science. Making high-flux membranes with carbon nanotubes. *Science*, **2006**, 312, 1003-4	33.3	179
218	Accelerating applications of metal-organic frameworks for gas adsorption and separation by computational screening of materials. *Langmuir*, **2012**, 28, 14114-28	4	178
217	Screening Metal□Organic Framework Materials for Membrane-based Methane/Carbon Dioxide Separations. *Journal of Physical Chemistry C*, **2007**, 111, 14055-14059	3.8	173
216	Understanding macroscopic diffusion of adsorbed molecules in crystalline nanoporous materials via atomistic simulations. *Accounts of Chemical Research*, **2006**, 39, 403-11	24.3	171
215	Molecular Dynamics Simulations of Self-Diffusivities, Corrected Diffusivities, and Transport Diffusivities of Light Gases in Four Silica Zeolites To Assess Influences of Pore Shape and Connectivity. *Journal of Physical Chemistry A*, **2003**, 107, 10132-10141	2.8	169
214	Adsorption and separation of hydrogen isotopes in carbon nanotubes: Multicomponent grand canonical Monte Carlo simulations. *Journal of Chemical Physics*, **2002**, 116, 814-824	3.9	167
213	Finding MOFs for highly selective CO2/N2 adsorption using materials screening based on efficient assignment of atomic point charges. *Journal of the American Chemical Society*, **2012**, 134, 4313-23	16.4	165
212	Quantifying large effects of framework flexibility on diffusion in MOFs: CH4 and CO2 in ZIF-8. *ChemPhysChem*, **2012**, 13, 3449-52	3.2	164
211	Selecting metal organic frameworks as enabling materials in mixed matrix membranes for high efficiency natural gas purification. *Energy and Environmental Science*, **2010**, 3, 343	35.4	159
210	Highly tunable molecular sieving and adsorption properties of mixed-linker zeolitic imidazolate frameworks. *Journal of the American Chemical Society*, **2015**, 137, 4191-7	16.4	155
209	Role of amine structure on carbon dioxide adsorption from ultradilute gas streams such as ambient air. *ChemSusChem*, **2012**, 5, 2058-64	8.3	151
208	Efficient methods for screening of metal organic framework membranes for gas separations using atomically detailed models. *Langmuir*, **2009**, 25, 11786-95	4	149
207	Monte Carlo Simulation of Single- and Binary-Component Adsorption of CO2, N2, and H2 in Zeolite Na-4A. *Energy & Fuels*, **2003**, 17, 977-983	4.1	147
206	Direct Air Capture of CO2 Using Amine Functionalized MIL-101(Cr). *ACS Sustainable Chemistry and Engineering*, **2016**, 4, 5761-5768	8.3	131

205	Role of Lewis and Brønsted Acid Sites in the Dehydration of Glycerol over Niobia. *ACS Catalysis*, **2014**, 4, 3180-3192	13.1	124
204	Direct Tests of the Darken Approximation for Molecular Diffusion in Zeolites Using Equilibrium Molecular Dynamics. *Journal of Physical Chemistry B*, **2001**, 105, 3151-3154	3.4	124
203	Temperature and Loading-Dependent Diffusion of Light Hydrocarbons in ZIF-8 as Predicted Through Fully Flexible Molecular Simulations. *Journal of the American Chemical Society*, **2015**, 137, 15760-71	16.4	121
202	Rational Tuning of Water Vapor and CO2Adsorption in Highly Stable Zr-Based MOFs. *Journal of Physical Chemistry C*, **2012**, 116, 23526-23532	3.8	121
201	Crystal-Size-Dependent Structural Transitions in Nanoporous Crystals: Adsorption-Induced Transitions in ZIF-8. *Journal of Physical Chemistry C*, **2014**, 118, 20727-20733	3.8	118
200	Carbon dioxide and methane transport in DDR zeolite: insights from molecular simulations into carbon dioxide separations in small pore zeolites. *Journal of the American Chemical Society*, **2009**, 131, 7896-904	16.4	115
199	Analysis of Equilibrium-Based TSA Processes for Direct Capture of CO2 from Air. *Industrial & Engineering Chemistry Research*, **2012**, 51, 8631-8645	3.9	112
198	Adsorption and Diffusion of Small Alcohols in Zeolitic Imidazolate Frameworks ZIF-8 and ZIF-90. *Journal of Physical Chemistry C*, **2013**, 117, 3169-3176	3.8	111
197	Structure and mobility of metal clusters in MOFs: Au, Pd, and AuPd clusters in MOF-74. *Journal of the American Chemical Society*, **2012**, 134, 12807-16	16.4	109
196	Prediction of CO2 Adsorption Properties in Zeolites Using Force Fields Derived from Periodic Dispersion-Corrected DFT Calculations. *Journal of Physical Chemistry C*, **2012**, 116, 10692-10701	3.8	107
195	Recent developments in first-principles force fields for molecules in nanoporous materials. *Journal of Materials Chemistry A*, **2014**, 2, 274-291	13	104
194	Structures of glycine, enantiopure alanine, and racemic alanine adlayers on Cu(110) and Cu(100) surfaces. *Journal of Physical Chemistry B*, **2005**, 109, 16764-73	3.4	100
193	How Reproducible Are Isotherm Measurements in Metal□Organic Frameworks?. *Chemistry of Materials*, **2017**, 29, 10487-10495	9.6	98
192	Facet-Specific Stability of ZIF-8 in the Presence of Acid Gases Dissolved in Aqueous Solutions. *Chemistry of Materials*, **2016**, 28, 6960-6967	9.6	96
191	A Comprehensive Set of High-Quality Point Charges for Simulations of Metal□Organic Frameworks. *Chemistry of Materials*, **2016**, 28, 785-793	9.6	95
190	Molecular Simulations and Theoretical Predictions for Adsorption and Diffusion of CH4/H2 and CO2/CH4 Mixtures in ZIFs. *Journal of Physical Chemistry C*, **2011**, 115, 12560-12566	3.8	95
189	Light isotope separation in carbon nanotubes through quantum molecular sieving. *Physical Review B*, **2001**, 63,	3.3	93
188	Identification of Metal□Organic Framework Materials for Adsorption Separation of Rare Gases: Applicability of Ideal Adsorbed Solution Theory (IAST) and Effects of Inaccessible Framework Regions. *Journal of Physical Chemistry C*, **2012**, 116, 13183-13195	3.8	92

187	High-throughput screening of metal-organic frameworks for CO2 separation. *ACS Combinatorial Science*, **2012**, 14, 263-7	3.9	91
186	Accurate Treatment of Electrostatics during Molecular Adsorption in Nanoporous Crystals without Assigning Point Charges to Framework Atoms. *Journal of Physical Chemistry C*, **2011**, 115, 4824-4836	3.8	91
185	Propane dehydrogenation catalyzed by gallosilicate MFI zeolites with perturbed acidity. *Journal of Catalysis*, **2017**, 345, 113-123	7.3	86
184	CO2 capture via adsorption in amine-functionalized sorbents. *Current Opinion in Chemical Engineering*, **2016**, 12, 82-90	5.4	84
183	Computational Characterization of Defects in Metal-Organic Frameworks: Spontaneous and Water-Induced Point Defects in ZIF-8. *Journal of Physical Chemistry Letters*, **2016**, 7, 459-64	6.4	82
182	Structural and Mechanistic Differences in Mixed-Linker Zeolitic Imidazolate Framework Synthesis by Solvent Assisted Linker Exchange and de Novo Routes. *Journal of the American Chemical Society*, **2017**, 139, 5906-5915	16.4	81
181	MOF stability and gas adsorption as a function of exposure to water, humid air, SO2, and NO2. *Microporous and Mesoporous Materials*, **2013**, 173, 86-91	5.3	81
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179	Propane Dehydrogenation over Alumina-Supported Iron/Phosphorus Catalysts: Structural Evolution of Iron Species Leading to High Activity and Propylene Selectivity. *ACS Catalysis*, **2016**, 6, 5673-5683	12.1	79
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177	Molecular chemisorption on open metal sites in Cu(3)(benzenetricarboxylate)(2): A spatially periodic density functional theory study. *Journal of Chemical Physics*, **2010**, 133, 094509	3.9	76
176	Ab initio lattice-gas modeling of interstitial hydrogen diffusion in CuPd alloys. *Physical Review B*, **2005**, 71,	3.3	76
175	Pore size analysis of >250,000 hypothetical zeolites. *Physical Chemistry Chemical Physics*, **2011**, 13, 5053-60	3.6	75
174	Large-Scale Refinement of Metal–Organic Framework Structures Using Density Functional Theory. *Chemistry of Materials*, **2017**, 29, 2521-2528	9.6	74
173	Developing chiral surfaces for enantioselective chemical processing. *AICHE Journal*, **2009**, 55, 2484-2490	3.6	72
172	Interactions of SO2-Containing Acid Gases with ZIF-8: Structural Changes and Mechanistic Investigations. *Journal of Physical Chemistry C*, **2016**, 120, 27221-27229	3.8	71
171	Comparisons of diffusive and viscous contributions to transport coefficients of light gases in single-walled carbon nanotubes. *Molecular Simulation*, **2005**, 31, 643-649	2	71
170	Predictive assessment of surface resistances in zeolite membranes using atomically detailed models. *Journal of Physical Chemistry B*, **2005**, 109, 7237-44	3.4	65

169	Methods for Computing Accurate Atomic Spin Moments for Collinear and Noncollinear Magnetism in Periodic and Nonperiodic Materials. *Journal of Chemical Theory and Computation*, **2011**, 7, 4146-64	6.4	62
168	Atomically Detailed Models of the Effect of Thermal Roughening on the Enantiospecificity of Naturally Chiral Platinum Surfaces. *Langmuir*, **2002**, 18, 3737-3748	4	62
167	Molecular dynamics simulation of framework flexibility effects on noble gas diffusion in HKUST-1 and ZIF-8. *Microporous and Mesoporous Materials*, **2014**, 194, 190-199	5.3	61
166	Synergistic Effects of Water and SO2 on Degradation of MIL-125 in the Presence of Acid Gases. *Journal of Physical Chemistry C*, **2016**, 120, 27230-27240	3.8	59
165	First principles derived, transferable force fields for CO2 adsorption in Na-exchanged cationic zeolites. *Physical Chemistry Chemical Physics*, **2013**, 15, 12882-94	3.6	58
164	Hierarchical Ga-MFI Catalysts for Propane Dehydrogenation. *Chemistry of Materials*, **2017**, 29, 7213-7222	9.6	58
163	Surface interactions of C and C(3) polyols with Al2O3 and the role of coadsorbed water. *Langmuir*, **2013**, 29, 581-93	4	58
162	Examining the accuracy of ideal adsorbed solution theory without curve-fitting using transition matrix Monte Carlo simulations. *Langmuir*, **2007**, 23, 6431-7	4	58
161	Predicting Single-Component Permeance through Macroscopic Zeolite Membranes from Atomistic Simulations. *Industrial & Engineering Chemistry Research*, **2000**, 39, 3737-3746	3.9	56
160	Monolith-Supported Amine-Functionalized Mg(dobpdc) Adsorbents for CO Capture. *ACS Applied Materials & Interfaces*, **2017**, 9, 17042-17050	9.5	53
159	Benchmarking density functional theory predictions of framework structures and properties in a chemically diverse test set of metal-organic frameworks. *Journal of Materials Chemistry A*, **2015**, 3, 22432-22440	13	49
158	CO2 Dynamics in Pure and Mixed-Metal MOFs with Open Metal Sites. *Journal of Physical Chemistry C*, **2017**, 121, 25778-25787	3.8	49
157	Density Functional Theory Study of H and CO Adsorption on Alkali-Promoted Mo2C Surfaces. *Journal of Physical Chemistry C*, **2011**, 115, 6870-6876	3.8	49
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155	Acid Gas Stability of Zeolitic Imidazolate Frameworks: Generalized Kinetic and Thermodynamic Characteristics. *Chemistry of Materials*, **2018**, 30, 4089-4101	9.6	49
154	Prediction of Water Adsorption in Copper-Based Metal-Organic Frameworks Using Force Fields Derived from Dispersion-Corrected DFT Calculations. *Journal of Physical Chemistry C*, **2013**, 117, 7519-7525	3.8	46
153	Using first-principles calculations to accelerate materials discovery for hydrogen purification membranes by modeling amorphous metals. *Energy and Environmental Science*, **2008**, 1, 175	35.4	46
152	Identification of High-CO2-Capacity Cationic Zeolites by Accurate Computational Screening. *Chemistry of Materials*, **2016**, 28, 3887-3896	9.6	46

151	Efficient and Accurate Methods for Characterizing Effects of Framework Flexibility on Molecular Diffusion in Zeolites: CH4 Diffusion in Eight Member Ring Zeolites. *Journal of Physical Chemistry C*, **2013**, 117, 13462-13473	3.8	45
150	Enantiospecific adsorption of chiral hydrocarbons on naturally chiral Pt and Cu surfaces. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **1999**, 17, 1700-1704	2.9	45
149	Screening of Copper Open Metal Site MOFs for Olefin/Paraffin Separations Using DFT-Derived Force Fields. *Journal of Physical Chemistry C*, **2016**, 120, 23044-23054	3.8	45
148	Control of Metal□Organic Framework Crystal Topology by Ligand Functionalization: Functionalized HKUST-1 Derivatives. *Crystal Growth and Design*, **2014**, 14, 6122-6128	3.5	43
147	The Physico-chemical Properties of Cinchona Alkaloids Responsible for their Unique Performance in Chiral Catalysis. *Topics in Catalysis*, **2008**, 48, 120-127	2.3	43
146	Heat-Treatment of Defective UiO-66 from Modulated Synthesis: Adsorption and Stability Studies. *Journal of Physical Chemistry C*, **2017**, 121, 23471-23479	3.8	42
145	First-principles studies of chiral step reconstructions of Cu(100) by adsorbed glycine and alanine. *Journal of Chemical Physics*, **2006**, 124, 74703	3.9	42
144	Influences of concerted cluster diffusion on single-file diffusion of CF4 in AlPO4-5 and Xe in AlPO4-31. *Journal of Chemical Physics*, **2000**, 112, 817-824	3.9	42
143	Thin Hydrogen-Selective SAPO-34 Zeolite Membranes for Enhanced Conversion and Selectivity in Propane Dehydrogenation Membrane Reactors. *Chemistry of Materials*, **2016**, 28, 4397-4402	9.6	41
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141	Transition State Theory Methods To Measure Diffusion in Flexible Nanoporous Materials: Application to a Porous Organic Cage Crystal. *Journal of Physical Chemistry C*, **2016**, 120, 1110-1120	3.8	40
140	Flexibility of Ordered Surface Hydroxyls Influences the Adsorption of Molecules in Single-Walled Aluminosilicate Nanotubes. *Journal of Physical Chemistry Letters*, **2010**, 1, 1235-1240	6.4	40
139	Efficiently Exploring Adsorption Space to Identify Privileged Adsorbents for Chemical Separations of a Diverse Set of Molecules. *ChemSusChem*, **2018**, 11, 1567-1575	8.3	39
138	Effects of Intrinsic Flexibility on Adsorption Properties of Metal-Organic Frameworks at Dilute and Nondilute Loadings. *ACS Applied Materials & Interfaces*, **2019**, 11, 31060-31068	9.5	39
137	High-Tc Layered Ferrielectric Crystals by Coherent Spinodal Decomposition. *ACS Nano*, **2015**, 9, 12365-73	16.7	39
136	Importance of Kinetics in Surface Alloying: A Comparison of the Diffusion Pathways of Pd and Ag Atoms on Cu(111). *Journal of Physical Chemistry C*, **2009**, 113, 12863-12869	3.8	39
135	Structure Elucidation of Mixed-Linker Zeolitic Imidazolate Frameworks by Solid-State (1)H CRAMPS NMR Spectroscopy and Computational Modeling. *Journal of the American Chemical Society*, **2016**, 138, 7325-36	16.4	39
134	Establishing upper bounds on CO2 swing capacity in sub-ambient pressure swing adsorption via molecular simulation of metal□organic frameworks. *Journal of Materials Chemistry A*, **2017**, 5, 12258-12265	13	38

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132	Understanding Structure, Metal Distribution, and Water Adsorption in Mixed-Metal MOF-74. *Journal of Physical Chemistry C*, **2017**, 121, 627-635	3.8	37
131	Insights into the Stability of Zeolitic Imidazolate Frameworks in Humid Acidic Environments from First-Principles Calculations. *Journal of Physical Chemistry C*, **2018**, 122, 4339-4348	3.8	37
130	Efficient simulation of binary adsorption isotherms using transition matrix Monte Carlo. *Langmuir*, **2006**, 22, 709-16	4	37
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127	Temperature-regulated guest admission and release in microporous materials. *Nature Communications*, **2017**, 8, 15777	17.4	36
126	Liquid-Phase Multicomponent Adsorption and Separation of Xylene Mixtures by Flexible MIL-53 Adsorbents. *Journal of Physical Chemistry C*, **2018**, 122, 386-397	3.8	36
125	Metal-organic frameworks: a porous maze. *Nature Chemistry*, **2011**, 3, 429-30	17.6	36
124	Computational Prediction of Metal Organic Frameworks Suitable for Molecular Infiltration as a Route to Development of Conductive Materials. *Journal of Physical Chemistry Letters*, **2015**, 6, 1586-91	6.4	35
123	Effect of Framework Flexibility on C8 Aromatic Adsorption at High Loadings in Metal□Organic Frameworks. *Journal of Physical Chemistry C*, **2016**, 120, 370-376	3.8	35
122	How Well Do Approximate Models of Adsorption-Based CO2 Capture Processes Predict Results of Detailed Process Models?. *Industrial & Engineering Chemistry Research*, **2020**, 59, 7097-7108	3.9	35
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120	Formation Mechanisms and Defect Engineering of Imine-Based Porous Organic Cages. *Chemistry of Materials*, **2018**, 30, 262-272	9.6	34
119	Osmotic ensemble methods for predicting adsorption-induced structural transitions in nanoporous materials using molecular simulations. *Journal of Chemical Physics*, **2011**, 134, 184103	3.9	33
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109	Multiscale models of sweep gas and porous support effects on zeolite membranes. *AICHE Journal*, **2005**, 51, 867-877	3.6	26
108	Characterization of the Thermodynamic Stability of Solvated Metal Organic Framework Polymorphs Using Molecular Simulations. *Journal of Physical Chemistry C*, **2013**, 117, 20636-20642	3.8	25
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101	Engineering Porous Organic Cage Crystals with Increased Acid Gas Resistance. *Chemistry - A European Journal*, **2016**, 22, 10743-7	4.8	24
100	Does repeat synthesis in materials chemistry obey a power law?. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 877-882	11.5	23
99	Tuning Binding Tendencies of Small Molecules in Metal Organic Frameworks with Open Metal Sites by Metal Substitution and Linker Functionalization. *Journal of Physical Chemistry C*, **2018**, 122, 27486-27494	3.8	23
98	Selecting Adsorbents to Separate Diverse Near-Azeotropic Chemicals. *Journal of Physical Chemistry C*, **2020**, 124, 3664-3670	3.8	22

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96	Computational Screening of Functionalized UiO-66 Materials for Selective Contaminant Removal from Air. *Journal of Physical Chemistry C*, **2017**, 121, 20396-20406	3.8	22
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94	Pt thin films on the polar LaAlO3(100) surface: A first-principles study. *Physical Review B*, **2006**, 73,	3.3	22
93	Analysis of Binary Transport Diffusivities and Self-Diffusivities in a Lattice Model for Silicalite. *Langmuir*, **2002**, 18, 7393-7400	4	22
92	A Collection of More than 900 Gas Mixture Adsorption Experiments in Porous Materials from Literature Meta-Analysis. *Industrial & Engineering Chemistry Research*, **2021**, 60, 639-651	3.9	22
91	Stability of Zeolitic Imidazolate Frameworks in NO2. *Journal of Physical Chemistry C*, **2019**, 123, 2336-2346	3.8	22
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89	Acid Gas Adsorption on Metal-Organic Framework Nanosheets as a Model of an "All-Surface" Material. *Journal of Chemical Theory and Computation*, **2017**, 13, 1341-1350	6.4	20
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87	First principles assessment of perovskite dopants for proton conductors with chemical stability and high conductivity. *RSC Advances*, **2013**, 3, 3333	3.7	20
86	Atomically detailed simulations of surface resistances to transport of CH4, CF4, and C2H6 through silicalite membranes. *Microporous and Mesoporous Materials*, **2008**, 107, 286-295	5.3	20
85	Screening Diffusion of Small Molecules in Flexible Zeolitic Imidazolate Frameworks Using a DFT-Parameterized Force Field. *Journal of Physical Chemistry C*, **2019**, 123, 9153-9167	3.8	19
84	Modeling Diffusion of Linear Hydrocarbons in Silica Zeolite LTA Using Transition Path Sampling. *Journal of Physical Chemistry C*, **2015**, 119, 15643-15653	3.8	19
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