David S Sholl

List of Publications by Year
in descending order

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246 papers	21,920 citations	9756 73 h-index	11030 137 g-index
249 all docs	249 docs citations	249 times ranked	16499 citing authors

#	Article	IF	Citations
1	Seven chemical separations to change the world. Nature, 2016, 532, 435-437.	13.7	2,758
2	Can Metalâ€“Organic Framework Materials Play a Useful Role in Largeâ€Scale Carbon Dioxide Separations?. ChemSusChem, 2010, 3, 879-891.	3.6	556
3	Computation-Ready, Experimental Metalâ€“Organic Frameworks: A Tool To Enable High-Throughput Screening of Nanoporous Crystals. Chemistry of Materials, 2014, 26, 6185-6192.	3.2	524
4	Chiral selection on inorganic crystalline surfaces. Nature Materials, 2003, 2, 367-374.	13.3	439
5	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, 15760-15768.	1.2	412
6	Advances, Updates, and Analytics for the Computation-Ready, Experimental Metalâ€“Organic Framework Database: CoRE MOF 2019. Journal of Chemical & Engineering Data, 2019, 64, 5985-5998.	1.0	372
7	Chemically Meaningful Atomic Charges That Reproduce the Electrostatic Potential in Periodic and Nonperiodic Materials. Journal of Chemical Theory and Computation, 2010, 6, 2455-2468.	2.3	365
8	From water to organics in membrane separations. Nature Materials, 2017, 16, 276-279.	13.3	358
9	Nanoscale design to enable the revolution in renewable energy. Energy and Environmental Science, 2009, 2, 559.	15.6	348
10	Predicting multicomponent adsorption: 50 years of the ideal adsorbed solution theory. AICHE Journal, 2015, 61, 2757-2762.	1.8	317
11	The materials genome in action: identifying the performance limits for methane storage. Energy and Environmental Science, 2015, 8, 1190-1199.	15.6	314
12	Defects in Metalâ€“Organic Frameworks: Challenge or Opportunity?. Journal of Physical Chemistry Letters, 2015, 6, 3437-3444.	2.1	290
13	UltemÂ®/ZIF-8 mixed matrix hollow fiber membranes for CO2/N2 separations. Journal of Membrane Science, 2012, 401-402, 76-82.	4.1	289
14	Progress, Opportunities, and Challenges for Applying Atomically Detailed Modeling to Molecular Adsorption and Transport in Metalâ^'Organic Framework Materials. Industrial & Engineering Chemistry Research, 2009, 48, 2355-2371.	1.8	283
15	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, 2844-2867.	2.3	282
16	Exploring the Framework Hydrophobicity and Flexibility of ZIF-8: From Biofuel Recovery to Hydrocarbon Separations. Journal of Physical Chemistry Letters, 2013, 4, 3618-3622.	2.1	277
17	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, 7528-7539.	6.6	273
18	Modification of the Mg/DOBDC MOF with Amines to Enhance CO₂ Adsorption from Ultradilute Gases. Journal of Physical Chemistry Letters, 2012, 3, 1136-1141.	2.1	273

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19	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.	1.2	211
20	Direct Air Capture of CO₂ Using Amine Functionalized MIL-101(Cr). ACS Sustainable Chemistry and Engineering, 2016, 4, 5761-5768.	3.2	210
21	Naturally Chiral Metal Surfaces as Enantiospecific Adsorbents. Journal of Physical Chemistry B, 2001, 105, 4771-4782.	1.2	203
22	Accelerating Applications of Metalâ€“Organic Frameworks for Gas Adsorption and Separation by Computational Screening of Materials. Langmuir, 2012, 28, 14114-14128.	1.6	202
23	MATERIALS SCIENCE: Making High-Flux Membranes with Carbon Nanotubes. Science, 2006, 312, 1003-1004.	6.0	195
24	Understanding Macroscopic Diffusion of Adsorbed Molecules in Crystalline Nanoporous Materials via Atomistic Simulations. Accounts of Chemical Research, 2006, 39, 403-411.	7.6	193
25	Highly Tunable Molecular Sieving and Adsorption Properties of Mixed-Linker Zeolitic Imidazolate Frameworks. Journal of the American Chemical Society, 2015, 137, 4191-4197.	6.6	192
26	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, 4313-4323.	6.6	187
27	Screening Metalâ"Organic Framework Materials for Membrane-based Methane/Carbon Dioxide Separations. Journal of Physical Chemistry C, 2007, 111, 14055-14059.	1.5	186
28	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.	1.1	185
29	Quantifying Large Effects of Framework Flexibility on Diffusion in MOFs: CH₄ and CO₂ in ZIFâ€8. ChemPhysChem, 2012, 13, 3449-3452.	1.0	185
30	Role of Amine Structure on Carbon Dioxide Adsorption from Ultradilute Gas Streams such as Ambient Air. ChemSusChem, 2012, 5, 2058-2064.	3.6	180
31	Adsorption and separation of hydrogen isotopes in carbon nanotubes: Multicomponent grand canonical Monte Carlo simulations. Journal of Chemical Physics, 2002, 116, 814-824.	1.2	172
32	Selecting metal organic frameworks as enabling materials in mixed matrix membranes for high efficiency natural gas purification. Energy and Environmental Science, 2010, 3, 343.	15.6	172
33	Monte Carlo Simulation of Single- and Binary-Component Adsorption of CO2, N2, and H2in Zeolite Na-4A. Energy & Fuels, 2003, 17, 977-983.	2.5	165
34	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, 15760-15771.	6.6	164
35	Analysis of Equilibrium-Based TSA Processes for Direct Capture of CO₂ from Air. Industrial & Engineering Chemistry Research, 2012, 51, 8631-8645.	1.8	163
36	Role of Lewis and BrÃ¸nsted Acid Sites in the Dehydration of Glycerol over Niobia. ACS Catalysis, 2014, 4, 3180-3192.	5.5	163

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37	Efficient Methods for Screening of Metal Organic Framework Membranes for Gas Separations Using Atomically Detailed Models. Langmuir, 2009, 25, 11786-11795.	1.6	161
38	Crystal-Size-Dependent Structural Transitions in Nanoporous Crystals: Adsorption-Induced Transitions in ZIF-8. Journal of Physical Chemistry C, 2014, 118, 20727-20733.	1.5	145
39	A Comprehensive Set of High-Quality Point Charges for Simulations of Metalâ€“Organic Frameworks. Chemistry of Materials, 2016, 28, 785-793.	3.2	140
40	How Reproducible Are Isotherm Measurements in Metalâ€“Organic Frameworks?. Chemistry of Materials, 2017, 29, 10487-10495.	3.2	136
41	Adsorption and Diffusion of Small Alcohols in Zeolitic Imidazolate Frameworks ZIF-8 and ZIF-90. Journal of Physical Chemistry C, 2013, 117, 3169-3176.	1.5	135
42	Structure and Mobility of Metal Clusters in MOFs: Au, Pd, and AuPd Clusters in MOF-74. Journal of the American Chemical Society, 2012, 134, 12807-12816.	6.6	132
43	CO2 capture via adsorption in amine-functionalized sorbents. Current Opinion in Chemical Engineering, 2016, 12, 82-90.	3.8	132
44	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, 7896-7904.	6.6	130
45	Rational Tuning of Water Vapor and CO₂ Adsorption in Highly Stable Zr-Based MOFs. Journal of Physical Chemistry C, 2012, 116, 23526-23532.	1.5	129
46	Direct Tests of the Darken Approximation for Molecular Diffusion in Zeolites Using Equilibrium Molecular Dynamics. Journal of Physical Chemistry B, 2001, 105, 3151-3154.	1.2	128
47	Facet-Specific Stability of ZIF-8 in the Presence of Acid Gases Dissolved in Aqueous Solutions. Chemistry of Materials, 2016, 28, 6960-6967.	3.2	127
48	Recent developments in first-principles force fields for molecules in nanoporous materials. Journal of Materials Chemistry A, 2014, 2, 274-291.	5.2	126
49	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.	1.5	123
50	Computational Characterization of Defects in Metalâ€“Organic Frameworks: Spontaneous and Water-Induced Point Defects in ZIF-8. Journal of Physical Chemistry Letters, 2016, 7, 459-464.	2.1	119
51	Interactions of SO₂-Containing Acid Gases with ZIF-8: Structural Changes and Mechanistic Investigations. Journal of Physical Chemistry C, 2016, 120, 27221-27229.	1.5	115
52	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.	6.6	111
53	Propane dehydrogenation catalyzed by gallosilicate MFI zeolites with perturbed acidity. Journal of Catalysis, 2017, 345, 113-123.	3.1	111
54	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.	1.5	106

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55	High-Throughput Screening of Metalâ€“Organic Frameworks for CO₂ Separation. ACS Combinatorial Science, 2012, 14, 263-267.	3.8	106
56	Thermal, Oxidative and CO₂ Induced Degradation of Primary Amines Used for CO₂ Capture: Effect of Alkyl Linker on Stability. Journal of Physical Chemistry C, 2014, 118, 12302-12311.	1.5	103
57	Large-Scale Refinement of Metalâ^'Organic Framework Structures Using Density Functional Theory. Chemistry of Materials, 2017, 29, 2521-2528.	3.2	103
58	Identification of Metalâ€“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.	1.5	102
59	Structures of Glycine, Enantiopure Alanine, and Racemic Alanine Adlayers on Cu(110) and Cu(100) Surfaces. Journal of Physical Chemistry B, 2005, 109, 16764-16773.	1.2	101
60	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.	1.5	101
61	Light isotope separation in carbon nanotubes through quantum molecular sieving. Physical Review B, 2001, 63, .	1.1	100
62	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.	5.5	96
63	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.	2.2	94
64	Molecular chemisorption on open metal sites in Cu3(benzenetricarboxylate)2: A spatially periodic density functional theory study. Journal of Chemical Physics, 2010, 133, 094509.	1.2	87
65	Acid Gas Stability of Zeolitic Imidazolate Frameworks: Generalized Kinetic and Thermodynamic Characteristics. Chemistry of Materials, 2018, 30, 4089-4101.	3.2	86
66	Ab initiolattice-gas modeling of interstitial hydrogen diffusion in CuPd alloys. Physical Review B, 2005, 71, .	1.1	85
67	Computational identification of a metal organic framework for high selectivity membrane-based CO2/CH4 separations: Cu(hfipbb)(H2hfipbb)0.5. Physical Chemistry Chemical Physics, 2009, 11, 11389.	1.3	83
68	How Reproducible are Surface Areas Calculated from the BET Equation?. Advanced Materials, 2022, 34, .	11.1	82
69	Pore size analysis of >250â€‰000 hypothetical zeolites. Physical Chemistry Chemical Physics, 2011, 13, 5053.	1.3	81
70	Comparisons of diffusive and viscous contributions to transport coefficients of light gases in single-walled carbon nanotubes. Molecular Simulation, 2005, 31, 643-649.	0.9	79
71	Developing chiral surfaces for enantioselective chemical processing. AICHE Journal, 2009, 55, 2484-2490.	1.8	79
72	First principles derived, transferable force fields for CO2 adsorption in Na-exchanged cationic zeolites. Physical Chemistry Chemical Physics, 2013, 15, 12882.	1.3	79

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73	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.	1.5	79
74	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, 4146-4164.	2.3	77
75	Hierarchical Ga-MFI Catalysts for Propane Dehydrogenation. Chemistry of Materials, 2017, 29, 7213-7222.	3.2	77
76	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.	2.2	75
77	Heat-Treatment of Defective UiO-66 from Modulated Synthesis: Adsorption and Stability Studies. Journal of Physical Chemistry C, 2017, 121, 23471-23479.	1.5	73
78	Monolith-Supported Amine-Functionalized Mg₂(dobpdc) Adsorbents for CO₂ Capture. ACS Applied Materials & Interfaces, 2017, 9, 17042-17050.	4.0	71
79	Predictive Assessment of Surface Resistances in Zeolite Membranes Using Atomically Detailed Models. Journal of Physical Chemistry B, 2005, 109, 7237-7244.	1.2	70
80	High-T_c Layered Ferrielectric Crystals by Coherent Spinodal Decomposition. ACS Nano, 2015, 9, 12365-12373.	7.3	67
81	Atomically Detailed Models of the Effect of Thermal Roughening on the Enantiospecificity of Naturally Chiral Platinum Surfaces. Langmuir, 2002, 18, 3737-3748.	1.6	66
82	Surface Interactions of C₂ and C₃ Polyols with Î³-Al₂O₃ and the Role of Coadsorbed Water. Langmuir, 2013, 29, 581-593.	1.6	66
83	Examining the Accuracy of Ideal Adsorbed Solution Theory without Curve-Fitting Using Transition Matrix Monte Carlo Simulations. Langmuir, 2007, 23, 6431-6437.	1.6	65
84	Benchmarking density functional theory predictions of framework structures and properties in a chemically diverse test set of metalâ€“organic frameworks. Journal of Materials Chemistry A, 2015, 3, 22432-22440.	5.2	64
85	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.	1.5	61
86	Understanding Structure, Metal Distribution, and Water Adsorption in Mixed-Metal MOF-74. Journal of Physical Chemistry C, 2017, 121, 627-635.	1.5	61
87	Temperature-regulated guest admission and release in microporous materials. Nature Communications, 2017, 8, 15777.	5.8	60
88	Construction of an Anion-Pillared MOF Database and the Screening of MOFs Suitable for Xe/Kr Separation. ACS Applied Materials & Interfaces, 2021, 13, 11039-11049.	4.0	60
89	Density Functional Theory Study of H and CO Adsorption on Alkali-Promoted Mo₂C Surfaces. Journal of Physical Chemistry C, 2011, 115, 6870-6876.	1.5	59
90	CO₂ Dynamics in Pure and Mixed-Metal MOFs with Open Metal Sites. Journal of Physical Chemistry C, 2017, 121, 25778-25787.	1.5	59

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91	How Useful Are Common Simulants of Chemical Warfare Agents at Predicting Adsorption Behavior?. Journal of Physical Chemistry C, 2018, 122, 26061-26069.	1.5	58
92	Predicting Single-Component Permeance through Macroscopic Zeolite Membranes from Atomistic Simulations. Industrial & Engineering Chemistry Research, 2000, 39, 3737-3746.	1.8	57
93	Identification of High-CO₂-Capacity Cationic Zeolites by Accurate Computational Screening. Chemistry of Materials, 2016, 28, 3887-3896.	3.2	57
94	Prediction of Water Adsorption in Copper-Based Metalâ€“Organic Frameworks Using Force Fields Derived from Dispersion-Corrected DFT Calculations. Journal of Physical Chemistry C, 2013, 117, 7519-7525.	1.5	56
95	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.	1.5	55
96	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.	1.5	54
97	AZn2(BH4)5(A = Li, Na) and NaZn(BH4)3: Structural Studies. Journal of Physical Chemistry C, 2010, 114, 19127-19133.	1.5	53
98	Liquid-Phase Multicomponent Adsorption and Separation of Xylene Mixtures by Flexible MIL-53 Adsorbents. Journal of Physical Chemistry C, 2018, 122, 386-397.	1.5	52
99	Using first-principles calculations to accelerate materials discovery for hydrogen purification membranes by modeling amorphous metals. Energy and Environmental Science, 2008, 1, 175.	15.6	51
100	Thin Hydrogen-Selective SAPO-34 Zeolite Membranes for Enhanced Conversion and Selectivity in Propane Dehydrogenation Membrane Reactors. Chemistry of Materials, 2016, 28, 4397-4402.	3.2	51
101	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.	1.8	51
102	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.	0.9	50
103	Efficiently Exploring Adsorption Space to Identify Privileged Adsorbents for Chemical Separations of a Diverse Set of Molecules. ChemSusChem, 2018, 11, 1567-1575.	3.6	50
104	Effects of Intrinsic Flexibility on Adsorption Properties of Metalâ€“Organic Frameworks at Dilute and Nondilute Loadings. ACS Applied Materials & Interfaces, 2019, 11, 31060-31068.	4.0	50
105	Effect of Surface Structure of TiO₂ Nanoparticles on CO₂ Adsorption and SO₂ Resistance. ACS Sustainable Chemistry and Engineering, 2017, 5, 9295-9306.	3.2	49
106	Control of Metalâ€“Organic Framework Crystal Topology by Ligand Functionalization: Functionalized HKUST-1 Derivatives. Crystal Growth and Design, 2014, 14, 6122-6128.	1.4	48
107	Propane Dehydrogenation over In₂O₃â€“Ga₂O₃â€“Al₂O₃ Mixed Oxides. ChemCatChem, 2016, 8, 214-221.	1.8	48
108	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.	1.8	48

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109	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.	1.5	47
110	Moving Beyond Adsorption Capacity in Design of Adsorbents for CO₂ Capture from Ultradilute Feeds: Kinetics of CO₂ Adsorption in Materials with Stepped Isotherms. Industrial & Engineering Chemistry Research, 2019, 58, 366-377.	1.8	47
111	Fingerprinting diverse nanoporous materials for optimal hydrogen storage conditions using meta-learning. Science Advances, 2021, 7, .	4.7	47
112	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.	1.2	46
113	The Physico-chemical Properties of Cinchona Alkaloids Responsible for their Unique Performance in Chiral Catalysis. Topics in Catalysis, 2008, 48, 120-127.	1.3	46
114	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.	1.5	46
115	Flexibility of Ordered Surface Hydroxyls Influences the Adsorption of Molecules in Single-Walled Aluminosilicate Nanotubes. Journal of Physical Chemistry Letters, 2010, 1, 1235-1240.	2.1	46
116	Computational Identification and Experimental Evaluation of Metalâ€“Organic Frameworks for Xylene Enrichment. Journal of Physical Chemistry C, 2016, 120, 12075-12082.	1.5	46
117	Structure Elucidation of Mixed-Linker Zeolitic Imidazolate Frameworks by Solid-State 1H CRAMPS NMR Spectroscopy and Computational Modeling. Journal of the American Chemical Society, 2016, 138, 7325-7336.	6.6	45
118	Thermal Fluctuations in the Structure of Naturally Chiral Pt surfaces. Topics in Catalysis, 2002, 18, 193-200.	1.3	44
119	First-principles studies of chiral step reconstructions of Cu(100) by adsorbed glycine and alanine. Journal of Chemical Physics, 2006, 124, 074703.	1.2	44
120	Establishing upper bounds on CO₂ swing capacity in sub-ambient pressure swing adsorption via molecular simulation of metalâ€“organic frameworks. Journal of Materials Chemistry A, 2017, 5, 12258-12265.	5.2	44
121	Formation Mechanisms and Defect Engineering of Imine-Based Porous Organic Cages. Chemistry of Materials, 2018, 30, 262-272.	3.2	44
122	Tuning the Structures of Metalâ€“Organic Frameworks via a Mixed-Linker Strategy for Ethylene/Ethane Kinetic Separation. Chemistry of Materials, 2020, 32, 3715-3722.	3.2	44
123	Butanol Separation from Humid CO₂-Containing Multicomponent Vapor Mixtures by Zeolitic Imidazolate Frameworks. ACS Sustainable Chemistry and Engineering, 2017, 5, 9467-9476.	3.2	41
124	Tuning the Wettability of Metalâ€“Organic Frameworks via Defect Engineering for Efficient Oil/Water Separation. ACS Applied Materials & Interfaces, 2020, 12, 34413-34422.	4.0	41
125	A porous maze. Nature Chemistry, 2011, 3, 429-430.	6.6	39
126	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, 1586-1591.	2.1	39

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127	Assessing the Impact of Point Defects on Molecular Diffusion in ZIF-8 Using Molecular Simulations. Journal of Physical Chemistry Letters, 2018, 9, 4037-4044.	2.1	39
128	Efficient Simulation of Binary Adsorption Isotherms Using Transition Matrix Monte Carlo. Langmuir, 2006, 22, 709-716.	1.6	38
129	Effect of Framework Flexibility on C₈ Aromatic Adsorption at High Loadings in Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2016, 120, 370-376.	1.5	38
130	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.	3.3	38
131	Interpretable Machine Learning-Based Predictions of Methane Uptake Isotherms in Metalâ€“Organic Frameworks. Chemistry of Materials, 2021, 33, 3543-3552.	3.2	38
132	Antiphase domain boundaries at the Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>(001) surface. Physical Review B, 2012, 85, .	1.1	37
133	DFT-Derived Force Fields for Modeling Hydrocarbon Adsorption in MIL-47(V). Langmuir, 2015, 31, 8453-8468.	1.6	37
134	Using first-principles calculations to predict surface resistances to H2 transport through metal alloy membranes. Journal of Membrane Science, 2007, 303, 162-172.	4.1	36
135	Osmotic ensemble methods for predicting adsorption-induced structural transitions in nanoporous materials using molecular simulations. Journal of Chemical Physics, 2011, 134, 184103.	1.2	36
136	Competitive Binding of Ethylene, Water, and Carbon Monoxide in Metalâ€“Organic Framework Materials with Open Cu Sites. Journal of Physical Chemistry C, 2018, 122, 8960-8966.	1.5	35
137	Stability of Zeolitic Imidazolate Frameworks in NO₂. Journal of Physical Chemistry C, 2019, 123, 2336-2346.	1.5	35
138	Brownian dynamics simulation of the motion of a rigid sphere in a viscous fluid very near a wall. Journal of Chemical Physics, 2000, 113, 9268-9278.	1.2	34
139	Tuning Binding Tendencies of Small Molecules in Metalâ€“Organic Frameworks with Open Metal Sites by Metal Substitution and Linker Functionalization. Journal of Physical Chemistry C, 2018, 122, 27486-27494.	1.5	34
140	DFT-based force field development for noble gas adsorption in metal organic frameworks. Journal of Materials Chemistry A, 2015, 3, 23539-23548.	5.2	33
141	The Effect of Aluminum Short-Range Ordering on Carbon Dioxide Adsorption in Zeolites. Journal of Physical Chemistry C, 2018, 122, 12332-12340.	1.5	33
142	Research Challenges in Avoiding â€œShowstoppersâ€•in Developing Materials for Large-Scale Energy Applications. Joule, 2017, 1, 208-211.	11.7	32
143	Determining Diffusion Coefficients of Chemical Warfare Agents in Metalâ€“Organic Frameworks. Journal of Physical Chemistry Letters, 2019, 10, 7823-7830.	2.1	32
144	A Database of Porous Rigid Amorphous Materials. Chemistry of Materials, 2020, 32, 8020-8033.	3.2	32

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145	Exemplar Mixtures for Studying Complex Mixture Effects in Practical Chemical Separations. Jacs Au, 2022, 2, 322-327.	3.6	32
146	Effect of correlated flights on particle mobilities during single-file diffusion. Physical Review E, 1997, 55, 7753-7756.	0.8	31
147	Quantitative assessment of hydrogen diffusion by activated hopping and quantum tunneling in ordered intermetallics. Physical Review B, 2005, 72, .	1.1	31
148	Engineering Porous Organic Cage Crystals with Increased Acid Gas Resistance. Chemistry - A European Journal, 2016, 22, 10743-10747.	1.7	31
149	Molecular Simulation of Capture of Sulfur-Containing Gases by Porous Aromatic Frameworks. Journal of Physical Chemistry C, 2018, 122, 18456-18467.	1.5	31
150	Self-diffusion and macroscopic diffusion of hydrogen in amorphous metals from first-principles calculations. Journal of Chemical Physics, 2009, 130, 244705.	1.2	30
151	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.	1.5	30
152	Computational Screening of MOFs and Zeolites for Direct Air Capture of Carbon Dioxide under Humid Conditions. Journal of Physical Chemistry C, 2021, 125, 24630-24639.	1.5	30
153	Characterization of the Thermodynamic Stability of Solvated Metalâ€“Organic Framework Polymorphs Using Molecular Simulations. Journal of Physical Chemistry C, 2013, 117, 20636-20642.	1.5	29
154	One-Step Synthesis of Zeolite Membranes Containing Catalytic Metal Nanoclusters. ACS Applied Materials & Interfaces, 2016, 8, 24671-24681.	4.0	29
155	Significant Temperature Dependence of the Isosteric Heats of Adsorption of Gases in Zeolites Demonstrated by Experiments and Molecular Simulations. Journal of Physical Chemistry C, 2019, 123, 20405-20412.	1.5	29
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