Berend Smit

List of Publications by Year in descending order

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		2213	3402
347	39,676	99	183
papers	citations	h-index	g-index

384	384	384	26778
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Making Molecules Vibrate: Interactive Web Environment for the Teaching of Infrared Spectroscopy. Journal of Chemical Education, 2022, 99, 561-569.	1.1	13
2	Data-Driven Matching of Experimental Crystal Structures and Gas Adsorption Isotherms of Metalâ€“Organic Frameworks. Journal of Chemical & Engineering Data, 2022, 67, 1743-1756.	1.0	6
3	Making the collective knowledge of chemistry open and machine actionable. Nature Chemistry, 2022, 14, 365-376.	6.6	34
4	Effects of Degrees of Freedom on Calculating Diffusion Properties in Nanoporous Materials. Journal of Chemical Theory and Computation, 2022, , .	2.3	8
5	Characterization of Chemisorbed Species and Active Adsorption Sites in Mgâ€“Al Mixed Metal Oxides for High-Temperature CO₂ Capture. Chemistry of Materials, 2022, 34, 3893-3901.	3.2	10
6	Pyrene-based metal organic frameworks: from synthesis to applications. Chemical Society Reviews, 2021, 50, 3143-3177.	18.7	126
7	AiiDAlab â€“ an ecosystem for developing, executing, and sharing scientific workflows. Computational Materials Science, 2021, 188, 110165.	1.4	40
8	Buffered Coordination Modulation as a Means of Controlling Crystal Morphology and Molecular Diffusion in an Anisotropic Metalâ€“Organic Framework. Journal of the American Chemical Society, 2021, 143, 5044-5052.	6.6	35
9	Enhanced Visible-Light-Driven Hydrogen Production through MOF/MOF Heterojunctions. ACS Applied Materials & Interfaces, 2021, 13, 14239-14247.	4.0	73
10	Multilevel screening of computationâ€ready, experimental metalâ€organic frameworks for natural gas purification. AICHE Journal, 2021, 67, e17279.	1.8	6
11	Toward smart carbon capture with machine learning. Cell Reports Physical Science, 2021, 2, 100396.	2.8	38
12	Bias free multiobjective active learning for materials design and discovery. Nature Communications, 2021, 12, 2312.	5.8	78
13	Using collective knowledge to assign oxidation states of metal cations in metalâ€“organic frameworks. Nature Chemistry, 2021, 13, 771-777.	6.6	35
14	Common workflows for computing material properties using different quantum engines. Npj Computational Materials, 2021, 7, .	3.5	10
15	A data-driven perspective on the colours of metalâ€“organic frameworks. Chemical Science, 2021, 12, 3587-3598.	3.7	16
16	Trends in atomistic simulation software usage [Article v1.0]. Living Journal of Computational Molecular Science, 2021, 3, .	2.2	7
17	Toward Optimal Photocatalytic Hydrogen Generation from Water Using Pyrene-Based Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2021, 13, 57118-57131.	4.0	16
18	Diversifying Databases of Metal Organic Frameworks for High-Throughput Computational Screening. ACS Applied Materials & Interfaces, 2021, 13, 61004-61014.	4.0	50

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19	Too Many Materials and Too Many Applications: An Experimental Problem Waiting for a Computational Solution. ACS Central Science, 2020, 6, 1890-1900.	5.3	63
20	The Role of Machine Learning in the Understanding and Design of Materials. Journal of the American Chemical Society, 2020, 142, 20273-20287.	6.6	179
21	Understanding the diversity of the metal-organic framework ecosystem. Nature Communications, 2020, 11, 4068.	5.8	282
22	Thermoelasticity of Flexible Organic Crystals from Quasi-harmonic Lattice Dynamics: The Case of Copper(II) Acetylacetonate. Journal of Physical Chemistry Letters, 2020, 11, 8543-8548.	2.1	15
23	From Isolated Porphyrin Ligands to Periodic Al-PMOF: A Comparative Study of the Optical Properties Using DFT/TDDFT. Journal of Physical Chemistry C, 2020, 124, 21751-21760.	1.5	11
24	Materials Cloud, a platform for open computational science. Scientific Data, 2020, 7, 299.	2.4	189
25	Charge Separation and Charge Carrier Mobility in Photocatalytic Metalâ€Organic Frameworks. Advanced Functional Materials, 2020, 30, 2003792.	7.8	64
26	Optical absorption properties of metalâ€“organic frameworks: solid state versus molecular perspective. Physical Chemistry Chemical Physics, 2020, 22, 19512-19521.	1.3	14
27	A novel integrated Cr(<scp>vi</scp>) adsorptionâ€“photoreduction system using MOF@polymer composite beads. Journal of Materials Chemistry A, 2020, 8, 9629-9637.	5.2	64
28	Big-Data Science in Porous Materials: Materials Genomics and Machine Learning. Chemical Reviews, 2020, 120, 8066-8129.	23.0	284
29	Sustainable Hydrogenation of Nitroarenes to Anilines with Highly Active inâ€situ Generated Copper Nanoparticles. ChemCatChem, 2020, 12, 2833-2839.	1.8	14
30	Taking lanthanides out of isolation: tuning the optical properties of metalâ€“organic frameworks. Chemical Science, 2020, 11, 4164-4170.	3.7	12
31	In Silico Discovery of Covalent Organic Frameworks for Carbon Capture. ACS Applied Materials & Interfaces, 2020, 12, 21559-21568.	4.0	43
32	Energy-based descriptors for photo-catalytically active metalâ€“organic framework discovery. Journal of Materials Chemistry A, 2020, 8, 4473-4482.	5.2	24
33	Metal-organic frameworks as kinetic modulators for branched selectivity in hydroformylation. Nature Communications, 2020, 11, 1059.	5.8	40
34	On the Electronic and Optical Properties of Metalâ€“Organic Frameworks: Case Study of MIL-125 and MIL-125-NH₂. Journal of Physical Chemistry C, 2020, 124, 4065-4072.	1.5	50
35	Geometric landscapes for material discovery within energyâ€“structureâ€“function maps. Chemical Science, 2020, 11, 5423-5433.	3.7	23
36	Insights into the Electronic Properties and Charge Transfer Mechanism of a Porphyrin Ruthenium-Based Metalâ€“Organic Framework. Chemistry of Materials, 2020, 32, 4194-4204.	3.2	31

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37	Carbon capture and storage: making fossil fuels great again?. Europhysics News, 2020, 51, 20-22.	0.1	6
38	Sim-to-real transfer reinforcement learning for control of thermal effects of an atmospheric pressure plasma jet. Plasma Sources Science and Technology, 2019, 28, 095019.	1.3	24
39	Preserving Porosity of Mesoporous Metalâ€“Organic Frameworks through the Introduction of Polymer Guests. Journal of the American Chemical Society, 2019, 141, 12397-12405.	6.6	68
40	Guest-dependent negative thermal expansion in a lanthanide-based metalâ€“organic framework. CrystEngComm, 2019, 21, 5292-5298.	1.3	4
41	Can Metalâ€“Organic Frameworks Be Used for Cannabis Breathalyzers?. ACS Applied Materials & Interfaces, 2019, 11, 34777-34786.	4.0	1
42	Applicability of Tail Corrections in the Molecular Simulations of Porous Materials. Journal of Chemical Theory and Computation, 2019, 15, 5635-5641.	2.3	30
43	Simulating Enhanced Methane Deliverable Capacity of Guest Responsive Pores in Intrinsically Flexible MOFs. Journal of Physical Chemistry Letters, 2019, 10, 5929-5934.	2.1	16
44	Building a Consistent and Reproducible Database for Adsorption Evaluation in Covalentâ€“Organic Frameworks. ACS Central Science, 2019, 5, 1663-1675.	5.3	89
45	Capturing chemical intuition in synthesis of metal-organic frameworks. Nature Communications, 2019, 10, 539.	5.8	153
46	Ab Initio Flexible Force Field for Metalâ€“Organic Frameworks Using Dummy Model Coordination Bonds. Journal of Chemical Theory and Computation, 2019, 15, 3666-3677.	2.3	9
47	Combined Nuclear Magnetic Resonance and Molecular Dynamics Study of Methane Adsorption in M₂(dobdc) Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2019, 123, 12286-12295.	1.5	18
48	DORI Reveals the Influence of Noncovalent Interactions on Covalent Bonding Patterns in Molecular Crystals Under Pressure. Journal of Physical Chemistry Letters, 2019, 10, 1482-1488.	2.1	15
49	Metal Substitution as the Method of Modifying Electronic Structure of Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2019, 141, 6271-6278.	6.6	137
50	Nucleobase pairing and photodimerization in a biologically derived metal-organic framework nanoreactor. Nature Communications, 2019, 10, 1612.	5.8	58
51	Pushing the limit of Cs incorporation into FAPbBr3 perovskite to enhance solar cells performances. APL Materials, 2019, 7, .	2.2	33
52	Automated Multiscale Approach To Predict Self-Diffusion from a Potential Energy Field. Journal of Chemical Theory and Computation, 2019, 15, 2127-2141.	2.3	20
53	Amine Dynamics in Diamine-Appended Mg₂(dobpdc) Metalâ€“Organic Frameworks. Journal of Physical Chemistry Letters, 2019, 10, 7044-7049.	2.1	18
54	Carbons with Regular Pore Geometry Yield Fundamental Insights into Supercapacitor Charge Storage. ACS Central Science, 2019, 5, 1813-1823.	5.3	44

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55	Data-driven design of metalâ€“organic frameworks for wet flue gas CO2 capture. Nature, 2019, 576, 253-256.	13.7	438
56	Evaluating Charge Equilibration Methods To Generate Electrostatic Fields in Nanoporous Materials. Journal of Chemical Theory and Computation, 2019, 15, 382-401.	2.3	70
57	Distinguishing Metalâ€“Organic Frameworks. Crystal Growth and Design, 2018, 18, 1738-1747.	1.4	74
58	Shedding Light on the Protonation States and Location of Protonated N Atoms of Adenine in Metalâ€“Organic Frameworks. Inorganic Chemistry, 2018, 57, 1888-1900.	1.9	21
59	Cutting Materials in Half: A Graph Theory Approach for Generating Crystal Surfaces and Its Prediction of 2D Zeolites. ACS Central Science, 2018, 4, 235-245.	5.3	36
60	Photocatalytic hydrogen generation from a visible-light responsive metalâ€“organic framework system: the impact of nickel phosphide nanoparticles. Journal of Materials Chemistry A, 2018, 6, 2476-2481.	5.2	94
61	Unexpected Diffusion Anisotropy of Carbon Dioxide in the Metalâ€“Organic Framework Zn₂(dobpdc). Journal of the American Chemical Society, 2018, 140, 1663-1673.	6.6	64
62	Lanthanide-based near-infrared emitting metalâ€“organic frameworks with tunable excitation wavelengths and high quantum yields. Chemical Communications, 2018, 54, 6816-6819.	2.2	25
63	Carbon capture and storage (CCS): the way forward. Energy and Environmental Science, 2018, 11, 1062-1176.	15.6	2,378
64	Text Mining Metalâ€“Organic Framework Papers. Journal of Chemical Information and Modeling, 2018, 58, 244-251.	2.5	43
65	Dualâ€Functional Photocatalysis: Concurrent Photocatalytic Hydrogen Generation and Dye Degradation Using MILâ€125â€NH₂ under Visible Light Irradiation (Adv. Funct. Mater. 52/2018). Advanced Functional Materials, 2018, 28, 1870373.	7.8	6
66	Biporous Metalâ€“Organic Framework with Tunable CO₂/CH₄ Separation Performance Facilitated by Intrinsic Flexibility. ACS Applied Materials & Interfaces, 2018, 10, 36144-36156.	4.0	33
67	Concurrent Photocatalytic Hydrogen Generation and Dye Degradation Using MILâ€125â€NH₂ under Visible Light Irradiation. Advanced Functional Materials, 2018, 28, 1806368.	7.8	110
68	Flat-Histogram Monte Carlo as an Efficient Tool To Evaluate Adsorption Processes Involving Rigid and Deformable Molecules. Journal of Chemical Theory and Computation, 2018, 14, 6149-6158.	2.3	16
69	Metalâ€Organic Framework Beads: Porous Metalâ€“Organic Framework@Polymer Beads for Iodine Capture and Recovery Using a Gasâ€Sparged Column (Adv. Funct. Mater. 30/2018). Advanced Functional Materials, 2018, 28, 1870211.	7.8	5
70	Anomalous Effects of Velocity Rescaling Algorithms: The Flying Ice Cube Effect Revisited. Journal of Chemical Theory and Computation, 2018, 14, 5262-5272.	2.3	66
71	High-Throughput Screening Approach for Nanoporous Materials Genome Using Topological Data Analysis: Application to Zeolites. Journal of Chemical Theory and Computation, 2018, 14, 4427-4437.	2.3	53
72	Generating carbon schwarzites via zeolite-templating. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E8116-E8124.	3.3	88

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73	Photocatalytic Hydrogen Generation from a Visible-Light-Responsive Metalâ€“Organic Framework System: Stability versus Activity of Molybdenum Sulfide Cocatalysts. ACS Applied Materials & Interfaces, 2018, 10, 30035-30039.	4.0	71
74	Porous Metalâ€“Organic Framework@Polymer Beads for Iodine Capture and Recovery Using a Gasâ€“Sparged Column. Advanced Functional Materials, 2018, 28, 1801596.	7.8	120
75	In Silico Design of 2D and 3D Covalent Organic Frameworks for Methane Storage Applications. Chemistry of Materials, 2018, 30, 5069-5086.	3.2	101
76	Improving the Mechanical Stability of Metalâ€“Organic Frameworks Using Chemical Caryatids. ACS Central Science, 2018, 4, 832-839.	5.3	67
77	A bi-porous metalâ€“organic framework with tuneable sorption performance facilitated by intrinsic flexibility. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e261-e261.	0.0	0
78	Distinguishing metalâ€“organic frameworks. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e152-e152.	0.0	0
79	Impact of the strength and spatial distribution of adsorption sites on methane deliverable capacity in nanoporous materials. Chemical Engineering Science, 2017, 159, 18-30.	1.9	26
80	Statistical mechanical model of gas adsorption in porous crystals with dynamic moieties. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E287-E296.	3.3	34
81	Rational Design of a Low-Cost, High-Performance Metalâ€“Organic Framework for Hydrogen Storage and Carbon Capture. Journal of Physical Chemistry C, 2017, 121, 1171-1181.	1.5	84
82	Adsorbate-induced lattice deformation in IRMOF-74 series. Nature Communications, 2017, 8, 13945.	5.8	34
83	Materials Genome in Action: Identifying the Performance Limits of Physical Hydrogen Storage. Chemistry of Materials, 2017, 29, 2844-2854.	3.2	169
84	Performance of van der Waals Corrected Functionals for Guest Adsorption in the M₂(dobdc) Metalâ€“Organic Frameworks. Journal of Physical Chemistry A, 2017, 121, 4139-4151.	1.1	41
85	Predicting Product Distribution of Propene Dimerization in Nanoporous Materials. ACS Catalysis, 2017, 7, 3940-3948.	5.5	7
86	Formation pathways of metalâ€“organic frameworks proceeding through partial dissolution of the metastable phase. CrystEngComm, 2017, 19, 3407-3413.	1.3	20
87	Translational and Rotational Motion of C8 Aromatics Adsorbed in Isotropic Porous Media (MOF-5): NMR Studies and MD Simulations. Journal of Physical Chemistry C, 2017, 121, 15456-15462.	1.5	25
88	Quantifying similarity of pore-geometry in nanoporous materials. Nature Communications, 2017, 8, 15396.	5.8	98
89	The Influence of Intrinsic Framework Flexibility on Adsorption in Nanoporous Materials. Journal of the American Chemical Society, 2017, 139, 5547-5557.	6.6	100
90	Mixed-linker UiO-66: structureâ€“property relationships revealed by a combination of high-resolution powder X-ray diffraction and density functional theory calculations. Physical Chemistry Chemical Physics, 2017, 19, 1551-1559.	1.3	47

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91	Force-Field Prediction of Materials Properties in Metal-Organic Frameworks. Journal of Physical Chemistry Letters, 2017, 8, 357-363.	2.1	172
92	Effects of Pore and Cage Topology on the Thermodynamics of n-Alkane Adsorption at BrÃ¸nsted Protons in Zeolites at High Temperature. Journal of Physical Chemistry C, 2017, 121, 1618-1638.	1.5	17
93	Uncovering the Local Magnesium Environment in the Metalâ€“Organic Framework Mg2(dobpdc) Using 25Mg NMR Spectroscopy. Journal of Physical Chemistry C, 2017, 121, 19938-19945.	1.5	16
94	Introduction: Carbon Capture and Separation. Chemical Reviews, 2017, 117, 9521-9523.	23.0	157
95	Metalâ€“Organic Frameworks Invert Molecular Reactivity: Lewis Acidic Phosphonium Zwitterions Catalyze the Aldol-Tishchenko Reaction. Journal of the American Chemical Society, 2017, 139, 18166-18169.	6.6	30
96	Accurate Characterization of the Pore Volume in Microporous Crystalline Materials. Langmuir, 2017, 33, 14529-14538.	1.6	155
97	Computational development of the nanoporous materials genome. Nature Reviews Materials, 2017, 2, .	23.3	123
98	Origin of the Strong Interaction between Polar Molecules and Copper(II) Paddle-Wheels in Metal Organic Frameworks. Journal of Physical Chemistry C, 2017, 121, 15135-15144.	1.5	23
99	In silico design and screening of hypothetical MOF-74 analogs and their experimental synthesis. Chemical Science, 2016, 7, 6263-6272.	3.7	69
100	Carbon Capture and Storage: introductory lecture. Faraday Discussions, 2016, 192, 9-25.	1.6	45
101	First-principles Hubbard U approach for small molecule binding in metal-organic frameworks. Journal of Chemical Physics, 2016, 144, 174104.	1.2	73
102	Force Field Development from Periodic Density Functional Theory Calculations for Gas Separation Applications Using Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2016, 120, 12590-12604.	1.5	95
103	Pre-Transition Effects Mediate Forces of Assembly between Transmembrane Proteins: The Orderphobic Effect. Biophysical Journal, 2016, 110, 567a.	0.2	1
104	Cutting the cost of carbon capture: a case for carbon capture and utilization. Faraday Discussions, 2016, 192, 391-414.	1.6	33
105	Modelling â€“ from molecules to mega-scale: general discussion. Faraday Discussions, 2016, 192, 493-509.	1.6	0
106	High-throughput computational screening of nanoporous adsorbents for CO₂ capture from natural gas. Molecular Systems Design and Engineering, 2016, 1, 175-188.	1.7	54
107	CCS â€“ A technology for now: general discussion. Faraday Discussions, 2016, 192, 125-151.	1.6	5
108	CCS â€“ A technology for the future: general discussion. Faraday Discussions, 2016, 192, 303-335.	1.6	4

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109	Effects of Zeolite Structural Confinement on Adsorption Thermodynamics and Reaction Kinetics for Monomolecular Cracking and Dehydrogenation of n-Butane. Journal of the American Chemical Society, 2016, 138, 4739-4756.	6.6	72
110	pyIAST: Ideal adsorbed solution theory (IAST) Python package. Computer Physics Communications, 2016, 200, 364-380.	3.0	186
111	Metalâ€“organic framework with optimally selective xenon adsorption and separation. Nature Communications, 2016, 7, ncomms11831.	5.8	325
112	Pre-transition effects mediate forces of assembly between transmembrane proteins. ELife, 2016, 5, e13150.	2.8	56
113	Nanoporous Materials Can Tune the Critical Point of a Pure Substance. Angewandte Chemie - International Edition, 2015, 54, 14349-14352.	7.2	16
114	A Fundamental Force Governing Protein Self-Assembly in Membranes. Biophysical Journal, 2015, 108, 241a.	0.2	0
115	Understanding Smallâ€Molecule Interactions in Metalâ€“Organic Frameworks: Coupling Experiment with Theory. Advanced Materials, 2015, 27, 5785-5796.	11.1	33
116	Computer-Aided Search for Materials to Store Natural Gas for Vehicles. Frontiers for Young Minds, 2015, 3, .	0.8	2
117	Adsorption Thermodynamics and Intrinsic Activation Parameters for Monomolecular Cracking of n-Alkanes on BrÃ¸nsted Acid Sites in Zeolites. Journal of Physical Chemistry C, 2015, 119, 10427-10438.	1.5	48
118	What Are the Best Materials To Separate a Xenon/Krypton Mixture?. Chemistry of Materials, 2015, 27, 4459-4475.	3.2	211
119	Screening Materials Relevant for Energy Technologies. Chimia, 2015, 69, 248-252.	0.3	5
120	Water adsorption in metalâ€“organic frameworks with openâ€metal sites. AICHE Journal, 2015, 61, 677-687.	1.8	37
121	The materials genome in action: identifying the performance limits for methane storage. Energy and Environmental Science, 2015, 8, 1190-1199.	15.6	314
122	A Fundamental Force that Regulates Nano-Clustering of Proteins in Biological Membranes. Biophysical Journal, 2015, 108, 18a.	0.2	0
123	PSIIâ€“LHCII Supercomplex Organizations in Photosynthetic Membrane by Coarse-Grained Simulation. Journal of Physical Chemistry B, 2015, 119, 3999-4008.	1.2	15
124	Small-Molecule Adsorption in Open-Site Metalâ€“Organic Frameworks: A Systematic Density Functional Theory Study for Rational Design. Chemistry of Materials, 2015, 27, 668-678.	3.2	248
125	Cooperative insertion of CO2 in diamine-appended metal-organic frameworks. Nature, 2015, 519, 303-308.	13.7	1,026
126	CO₂ induced phase transitions in diamine-appended metalâ€“organic frameworks. Chemical Science, 2015, 6, 5177-5185.	3.7	45

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127	Carbon capture turned upside down: high-temperature adsorption & low-temperature desorption (HALD). Energy and Environmental Science, 2015, 8, 2480-2491.	15.6	19
128	Systematic Tuning and Multifunctionalization of Covalent Organic Polymers for Enhanced Carbon Capture. Journal of the American Chemical Society, 2015, 137, 13301-13307.	6.6	202
129	Critical Factors Driving the High Volumetric Uptake of Methane in Cu₃(btc)₂. Journal of the American Chemical Society, 2015, 137, 10816-10825.	6.6	73
130	In Silico Discovery of High Deliverable Capacity Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2015, 119, 186-195.	1.5	54
131	The Grand Challenges in Carbon Capture, Utilization, and Storage. Frontiers in Energy Research, 2014, 2, .	1.2	54
132	Kinetically tuned dimensional augmentation as a versatile synthetic route towards robust metalâ€“organic frameworks. Nature Communications, 2014, 5, 5723.	5.8	332
133	Computational screening of porous metalâ€organic frameworks and zeolites for the removal of SO₂ and NO_x from flue gases. AICHE Journal, 2014, 60, 2314-2323.	1.8	112
134	Computational carbon capture. , 2014, , .		2
135	Small scale membrane mechanics. Biomechanics and Modeling in Mechanobiology, 2014, 13, 697-711.	1.4	29
136	In silico Design of Porous Polymer Networks: High-Throughput Screening for Methane Storage Materials. Journal of the American Chemical Society, 2014, 136, 5006-5022.	6.6	146
137	Design of a Metalâ€“Organic Framework with Enhanced Back Bonding for Separation of N₂ and CH₄. Journal of the American Chemical Society, 2014, 136, 698-704.	6.6	157
138	On the Flexibility of Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2014, 136, 2228-2231.	6.6	198
139	A hybrid absorptionâ€“adsorption method to efficiently capture carbon. Nature Communications, 2014, 5, 5147.	5.8	163
140	Toward a Materials Genome Approach for Ionic Liquids: Synthesis Guided by Ab Initio Property Maps. Journal of Physical Chemistry B, 2014, 118, 13609-13620.	1.2	19
141	Optimizing nanoporous materials for gas storage. Physical Chemistry Chemical Physics, 2014, 16, 5499.	1.3	76
142	Efficient Determination of Accurate Force Fields for Porous Materials Using ab Initio Total Energy Calculations. Journal of Physical Chemistry C, 2014, 118, 2693-2701.	1.5	23
143	Evaluating different classes of porous materials for carbon capture. Energy and Environmental Science, 2014, 7, 4132-4146.	15.6	186
144	Comprehensive study of carbon dioxide adsorption in the metalâ€“organic frameworks M₂(dobdc) (M = Mg, Mn, Fe, Co, Ni, Cu, Zn). Chemical Science, 2014, 5, 4569-4581.	3.7	342

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145	In Silico Design of Three-Dimensional Porous Covalent Organic Frameworks via Known Synthesis Routes and Commercially Available Species. Journal of Physical Chemistry C, 2014, 118, 23790-23802.	1.5	40
146	CO₂ Adsorption in Fe₂(dobdc): A Classical Force Field Parameterized from Quantum Mechanical Calculations. Journal of Physical Chemistry C, 2014, 118, 12230-12240.	1.5	45
147	Force-Field Development from Electronic Structure Calculations with Periodic Boundary Conditions: Applications to Gaseous Adsorption and Transport in Metalâ€“Organic Frameworks. Journal of Chemical Theory and Computation, 2014, 10, 1477-1488.	2.3	121
148	Reversible CO Binding Enables Tunable CO/H₂ and CO/N₂ Separations in Metalâ€“Organic Frameworks with Exposed Divalent Metal Cations. Journal of the American Chemical Society, 2014, 136, 10752-10761.	6.6	210
149	Understanding Trends in CO₂ Adsorption in Metalâ€“Organic Frameworks with Open-Metal Sites. Journal of Physical Chemistry Letters, 2014, 5, 861-865.	2.1	139
150	Redox chemistry and metalâ€“insulator transitions intertwined in a nano-porous material. Nature Communications, 2014, 5, 4032.	5.8	12
151	Understanding the effect of side groups in ionic liquids on carbon-capture properties: a combined experimental and theoretical effort. Physical Chemistry Chemical Physics, 2013, 15, 3264.	1.3	28
152	Molecular Simulation Study of the Competitive Adsorption of H₂O and CO₂ in Zeolite 13X. Langmuir, 2013, 29, 15936-15942.	1.6	109
153	Mapping of Functional Groups in Metal-Organic Frameworks. Science, 2013, 341, 882-885.	6.0	411
154	Modeling Methane Adsorption in Interpenetrating Porous Polymer Networks. Journal of Physical Chemistry C, 2013, 117, 20037-20042.	1.5	25
155	Lipid mediated packing of transmembrane helices â€“ a dissipative particle dynamics study. Soft Matter, 2013, 9, 2673.	1.2	14
156	Methane storage capabilities of diamond analogues. Physical Chemistry Chemical Physics, 2013, 15, 20937.	1.3	10
157	Evaluating mixture adsorption models using molecular simulation. AICHE Journal, 2013, 59, 3054-3064.	1.8	31
158	New materials for methane capture from dilute and medium-concentration sources. Nature Communications, 2013, 4, 1694.	5.8	111
159	Understanding CO₂ Dynamics in Metalâ€“Organic Frameworks with Open Metal Sites. Angewandte Chemie - International Edition, 2013, 52, 4410-4413.	7.2	160
160	On the Thermodynamics of Framework Breathing: A Free Energy Model for Gas Adsorption in MIL-53. Journal of Physical Chemistry C, 2013, 117, 11540-11554.	1.5	61
161	Large-Scale Screening of Zeolite Structures for CO₂ Membrane Separations. Journal of the American Chemical Society, 2013, 135, 7545-7552.	6.6	105
162	The Mechanism of Carbon Dioxide Adsorption in an Alkylamine-Functionalized Metalâ€“Organic Framework. Journal of the American Chemical Society, 2013, 135, 7402-7405.	6.6	208

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163	Mail-Order Metalâ€“Organic Frameworks (MOFs): Designing Isoreticular MOF-5 Analogues Comprising Commercially Available Organic Molecules. Journal of Physical Chemistry C, 2013, 117, 12159-12167.	1.5	64
164	Probing Adsorption Interactions in Metalâ€“Organic Frameworks using X-ray Spectroscopy. Journal of the American Chemical Society, 2013, 135, 18183-18190.	6.6	56
165	At Berkeley, we recycle everything but CO₂. , 2013, 3, 159-160.		1
166	CO2 Capture by Metalâ€“Organic Frameworks with van der Waals Density Functionals. Journal of Physical Chemistry A, 2012, 116, 4957-4964.	1.1	92
167	Understanding the Phase Behavior of Coarse-Grained Model Lipid Bilayers through Computational Calorimetry. Journal of Physical Chemistry B, 2012, 116, 1551-1569.	1.2	73
168	On the Equivalence of Schemes for Simulating Bilayers at Constant Surface Tension. Journal of Chemical Theory and Computation, 2012, 8, 404-417.	2.3	5
169	Ligand-Assisted Enhancement of CO₂ Capture in Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2012, 134, 6714-6719.	6.6	95
170	Monte Carlo Study on the Water Meniscus Condensation and Capillary Force in Atomic Force Microscopy. Journal of Physical Chemistry C, 2012, 116, 21923-21931.	1.5	36
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