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	Carbon Dioxide Capture: Prospects for New Materials. Angewandte Chemie - International Edition, 2010, 49, 6058-6082.	7.2	3,452
2	Carbon capture and storage (CCS): the way forward. Energy and Environmental Science, 2018, 11, 1062-1176.	15.6	2,378
3	Understanding Molecular Simulation. Computers in Physics, 1997, 11, 351-354.	0.6	1,063
4	Cooperative insertion of CO2 in diamine-appended metal-organic frameworks. Nature, 2015, 519, 303-308.	13.7	1,026
5	Molecular Simulations of Zeolites: Adsorption, Diffusion, and Shape Selectivity. Chemical Reviews, 2008, 108, 4125-4184.	23.0	655
6	In silico screening of carbon-capture materials. Nature Materials, 2012, 11, 633-641.	13.3	497
7	Towards a molecular understanding of shape selectivity. Nature, 2008, 451, 671-678.	13.7	479
8	Selective Binding of O₂ over N₂ in a Redoxâ€“Active Metalâ€“Organic Framework with Open Iron(II) Coordination Sites. Journal of the American Chemical Society, 2011, 133, 14814-14822.	6.6	470
9	Computer simulations of vaporâ€“liquid phase equilibria ofnâ€alkanes. Journal of Chemical Physics, 1995, 102, 2126-2140.	1.2	467
10	Metalâ^'Organic Frameworks as Adsorbents for Hydrogen Purification and Precombustion Carbon Dioxide Capture. Journal of the American Chemical Society, 2011, 133, 5664-5667.	6.6	465
11	Simulating the critical behaviour of complex fluids. Nature, 1993, 365, 330-332.	13.7	451
12	Molecular Dynamics Simulations. , 2002, , 63-107.		441
13	Data-driven design of metalâ€“organic frameworks for wet flue gas CO2 capture. Nature, 2019, 576, 253-256.	13.7	438
14	Monte Carlo Simulations. , 2002, , 23-61.		414
15	Mapping of Functional Groups in Metal-Organic Frameworks. Science, 2013, 341, 882-885.	6.0	411
16	Novel scheme to study structural and thermal properties of continuously deformable molecules. Journal of Physics Condensed Matter, 1992, 4, 3053-3076.	0.7	384
17	Effect of cholesterol on the structure of a phospholipid bilayer. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 3654-3658.	3.3	376
18	Why Clays Swell. Journal of Physical Chemistry B, 2002, 106, 12664-12667.	1.2	350

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19	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
20	Kinetically tuned dimensional augmentation as a versatile synthetic route towards robust metalâ€“organic frameworks. Nature Communications, 2014, 5, 5723.	5.8	332
21	Metalâ€“organic framework with optimally selective xenon adsorption and separation. Nature Communications, 2016, 7, ncomms11831.	5.8	325
22	United Atom Force Field for Alkanes in Nanoporous Materials. Journal of Physical Chemistry B, 2004, 108, 12301-12313.	1.2	314
23	The materials genome in action: identifying the performance limits for methane storage. Energy and Environmental Science, 2015, 8, 1190-1199.	15.6	314
24	Computer simulations in the Gibbs ensemble. Molecular Physics, 1989, 68, 931-950.	0.8	311
25	Ab initio carbon capture in open-site metalâ€“organic frameworks. Nature Chemistry, 2012, 4, 810-816.	6.6	310
26	Big-Data Science in Porous Materials: Materials Genomics and Machine Learning. Chemical Reviews, 2020, 120, 8066-8129.	23.0	284
27	Understanding the diversity of the metal-organic framework ecosystem. Nature Communications, 2020, 11, 4068.	5.8	282
28	Comparative Molecular Simulation Study of CO₂/N₂ and CH₄/N₂ Separation in Zeolites and Metalâ"Organic Frameworks. Langmuir, 2009, 25, 5918-5926.	1.6	276
29	What makes a polar liquid a liquid?. Physical Review Letters, 1993, 71, 3991-3994.	2.9	275
30	Molecular Simulation Studies of Separation of CO₂/N₂, CO₂/CH₄, and CH₄/N₂ by ZIFs. Journal of Physical Chemistry C, 2010, 114, 8515-8522.	1.5	266
31	Mesoscopic models of biological membranes. Physics Reports, 2006, 437, 1-54.	10.3	263
32	Understanding the Role of Sodium during Adsorption:Â A Force Field for Alkanes in Sodium-Exchanged Faujasites. Journal of the American Chemical Society, 2004, 126, 11377-11386.	6.6	255
33	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
34	Lithiumâ€Doped 3D Covalent Organic Frameworks: Highâ€Capacity Hydrogen Storage Materials. Angewandte Chemie - International Edition, 2009, 48, 4730-4733.	7.2	244
35	Commensurate â€˜freezingâ€™ of alkanes in the channels of a zeolite. Nature, 1995, 374, 42-44.	13.7	239
36	Simulation Studies of Protein-Induced Bilayer Deformations, and Lipid-Induced Protein Tilting, on a Mesoscopic Model for Lipid Bilayers with Embedded Proteins. Biophysical Journal, 2005, 88, 1778-1798.	0.2	234

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37	Computer Simulations of the Energetics and Siting of n-Alkanes in Zeolites. The Journal of Physical Chemistry, 1994, 98, 8442-8452.	2.9	223
38	What Are the Best Materials To Separate a Xenon/Krypton Mixture?. Chemistry of Materials, 2015, 27, 4459-4475.	3.2	211
39	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
40	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
41	Doping of Alkali, Alkaline-Earth, and Transition Metals in Covalent-Organic Frameworks for Enhancing CO₂ Capture by First-Principles Calculations and Molecular Simulations. ACS Nano, 2010, 4, 4225-4237.	7.3	206
42	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
43	On the Flexibility of Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2014, 136, 2228-2231.	6.6	198
44	Entropy effects during sorption of alkanes in zeolites. Chemical Society Reviews, 2002, 31, 185-194.	18.7	193
45	Direct simulation of phase equilibria of chain molecules. Journal of Physics Condensed Matter, 1992, 4, L255-L259.	0.7	190
46	Addressing Challenges of Identifying Geometrically Diverse Sets of Crystalline Porous Materials. Journal of Chemical Information and Modeling, 2012, 52, 308-318.	2.5	189
47	Materials Cloud, a platform for open computational science. Scientific Data, 2020, 7, 299.	2.4	189
48	Evaluating different classes of porous materials for carbon capture. Energy and Environmental Science, 2014, 7, 4132-4146.	15.6	186
49	pyIAST: Ideal adsorbed solution theory (IAST) Python package. Computer Physics Communications, 2016, 200, 364-380.	3.0	186
50	Phase Behavior of Model Lipid Bilayersâ€. Journal of Physical Chemistry B, 2005, 109, 6553-6563.	1.2	185
51	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
52	Calculation of the chemical potential in the Gibbs ensemble. Molecular Physics, 1989, 68, 951-958.	0.8	178
53	Force-Field Prediction of Materials Properties in Metal-Organic Frameworks. Journal of Physical Chemistry Letters, 2017, 8, 357-363.	2.1	172
54	Investigation of Surfactant Efficiency Using Dissipative Particle Dynamics. Langmuir, 2003, 19, 8195-8205.	1.6	170

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55	Materials Genome in Action: Identifying the Performance Limits of Physical Hydrogen Storage. Chemistry of Materials, 2017, 29, 2844-2854.	3.2	169
56	Molecular Simulations of Swelling Clay Minerals. Journal of Physical Chemistry B, 2004, 108, 7586-7596.	1.2	168
57	Grand canonical Monte Carlo simulations of chain molecules: adsorption isotherms of alkanes in zeolites. Molecular Physics, 1995, 85, 153-172.	0.8	167
58	Computer simulations of surfactant self-assembly. Langmuir, 1993, 9, 9-11.	1.6	164
59	Adsorption of Linear and Branched Alkanes in the Zeolite Silicalite-1. Journal of the American Chemical Society, 1998, 120, 5599-5600.	6.6	163
60	A hybrid absorptionâ€“adsorption method to efficiently capture carbon. Nature Communications, 2014, 5, 5147.	5.8	163
61	Understanding CO₂ Dynamics in Metalâ€“Organic Frameworks with Open Metal Sites. Angewandte Chemie - International Edition, 2013, 52, 4410-4413.	7.2	160
62	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
63	Introduction: Carbon Capture and Separation. Chemical Reviews, 2017, 117, 9521-9523.	23.0	157
64	Accurate Characterization of the Pore Volume in Microporous Crystalline Materials. Langmuir, 2017, 33, 14529-14538.	1.6	155
65	Hysteresis in Clay Swelling Induced by Hydrogen Bonding:â€‰ Accurate Prediction of Swelling States. Langmuir, 2006, 22, 1223-1234.	1.6	154
66	Capturing chemical intuition in synthesis of metal-organic frameworks. Nature Communications, 2019, 10, 539.	5.8	153
67	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
68	Force Field Parametrization through Fitting on Inflection Points in Isotherms. Physical Review Letters, 2004, 93, 088302.	2.9	144
69	Molecular Simulations of Lipid-Mediated Protein-Protein Interactions. Biophysical Journal, 2008, 95, 1851-1865.	0.2	143
70	Molecular simulation of loading-dependent diffusion in nanoporous materials using extended dynamically corrected transition state theory. Journal of Chemical Physics, 2005, 122, 224712.	1.2	142
71	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
72	Phase Behavior and Induced Interdigitation in Bilayers Studied with Dissipative Particle Dynamics. Journal of Physical Chemistry B, 2003, 107, 11491-11501.	1.2	138

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73	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
74	Simulating the Adsorption Isotherms of Methane, Ethane, and Propane in the Zeolite Silicalite. The Journal of Physical Chemistry, 1995, 99, 5597-5603.	2.9	133
75	Molecular Simulation of the Vapor-Liquid Coexistence Curve of Methanol. The Journal of Physical Chemistry, 1995, 99, 1831-1833.	2.9	131
76	Predicting Large CO₂ Adsorption in Aluminosilicate Zeolites for Postcombustion Carbon Dioxide Capture. Journal of the American Chemical Society, 2012, 134, 18940-18943.	6.6	129
77	Pyrene-based metal organic frameworks: from synthesis to applications. Chemical Society Reviews, 2021, 50, 3143-3177.	18.7	126
78	Molecular simulations in zeolitic process design. Chemical Engineering Science, 2003, 58, 557-568.	1.9	123
79	Computational development of the nanoporous materials genome. Nature Reviews Materials, 2017, 2, .	23.3	123
80	Energetics of n-Alkanes in Zeolites:â€‰ A Configurational-Bias Monte Carlo Investigation into Pore Size Dependence. Journal of the American Chemical Society, 1996, 118, 6753-6759.	6.6	122
81	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
82	Enhanced Adsorption Selectivity of Hydrogen/Methane Mixtures in Metalâ^'Organic Frameworks with Interpenetration: A Molecular Simulation Study. Journal of Physical Chemistry C, 2008, 112, 9854-9860.	1.5	120
83	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
84	Electrostatic analogy for surfactant assemblies. The Journal of Physical Chemistry, 1992, 96, 4077-4083.	2.9	114
85	Understanding the Loading Dependence of Self-Diffusion in Carbon Nanotubes. Physical Review Letters, 2005, 95, 044501.	2.9	114
86	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
87	New materials for methane capture from dilute and medium-concentration sources. Nature Communications, 2013, 4, 1694.	5.8	111
88	Concurrent Photocatalytic Hydrogen Generation and Dye Degradation Using MILâ€125â€NH₂ under Visible Light Irradiation. Advanced Functional Materials, 2018, 28, 1806368.	7.8	110
89	Phase behavior of monomeric mixtures and polymer solutions with soft interaction potentials. Journal of Chemical Physics, 2001, 114, 7644-7654.	1.2	109
90	Investigation of entropy effects during sorption of mixtures of alkanes in MFI zeolite. Chemical Engineering Journal, 2002, 88, 81-94.	6.6	109

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91	Molecular Simulation Study of the Competitive Adsorption of H₂O and CO₂ in Zeolite 13X. Langmuir, 2013, 29, 15936-15942.	1.6	109
92	Molecular Simulation of Loading Dependent Slow Diffusion in Confined Systems. Physical Review Letters, 2004, 93, 248301.	2.9	108
93	Parallel Monte Carlo simulations. Physical Review E, 1995, 51, 1560-1568.	0.8	106
94	Are pressure fluctuation-based equilibrium methods really worse than nonequilibrium methods for calculating viscosities?. Journal of Chemical Physics, 2009, 131, 246101.	1.2	105
95	Large-Scale Screening of Zeolite Structures for CO₂ Membrane Separations. Journal of the American Chemical Society, 2013, 135, 7545-7552.	6.6	105
96	Separation of Alkane Isomers by Exploiting Entropy Effects during Adsorption on Silicalite-1:â€‰ A Configurational-Bias Monte Carlo Simulation Study. Langmuir, 2001, 17, 1558-1570.	1.6	104
97	Understanding Diffusion in Nanoporous Materials. Physical Review Letters, 2006, 96, 044501.	2.9	104
98	Adsorption isotherms of water in Liâ€“, Naâ€“, and Kâ€“montmorillonite by molecular simulation. Journal of Chemical Physics, 2001, 115, 3322-3329.	1.2	102
99	In Silico Design of 2D and 3D Covalent Organic Frameworks for Methane Storage Applications. Chemistry of Materials, 2018, 30, 5069-5086.	3.2	101
100	The Influence of Intrinsic Framework Flexibility on Adsorption in Nanoporous Materials. Journal of the American Chemical Society, 2017, 139, 5547-5557.	6.6	100
101	Influence of isotherm inflection on diffusion in silicalite. Chemical Engineering Science, 1999, 54, 1751-1757.	1.9	99
102	Molecular Simulation of the DMPC-Cholesterol Phase Diagram. Journal of Physical Chemistry B, 2010, 114, 10451-10461.	1.2	99
103	Quantifying similarity of pore-geometry in nanoporous materials. Nature Communications, 2017, 8, 15396.	5.8	98
104	Simulating the Effect of Nonframework Cations on the Adsorption of Alkanes in MFI-type Zeolites. Journal of Physical Chemistry B, 2003, 107, 12088-12096.	1.2	95
105	Ligand-Assisted Enhancement of CO₂ Capture in Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2012, 134, 6714-6719.	6.6	95
106	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
107	Molecular-dynamics simulations of amphiphilic molecules at a liquid-liquid interface. Physical Review A, 1988, 37, 3431-3433.	1.0	94
108	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

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109	Adsorption and separation of linear and branched alkanes on carbon nanotube bundles from configurational-bias Monte Carlo simulation. Physical Review B, 2005, 72, .	1.1	93
110	CO2 Capture by Metalâ€“Organic Frameworks with van der Waals Density Functionals. Journal of Physical Chemistry A, 2012, 116, 4957-4964.	1.1	92
111	Molecular simulation of adsorption of short linear alkanes and their mixtures in silicalite. AICHE Journal, 1998, 44, 1756-1764.	1.8	90
112	Large-Scale Computational Screening of Zeolites for Ethane/Ethene Separation. Langmuir, 2012, 28, 11914-11919.	1.6	90
113	Incommensurate Diffusion in Confined Systems. Physical Review Letters, 2003, 90, 245901.	2.9	89
114	Building a Consistent and Reproducible Database for Adsorption Evaluation in Covalentâ€“Organic Frameworks. ACS Central Science, 2019, 5, 1663-1675.	5.3	89
115	Shape Selectivity in Hydrocarbon Conversion. Angewandte Chemie - International Edition, 2001, 40, 736-739.	7.2	88
116	Simulating Induced Interdigitation in Membranes. Biophysical Journal, 2004, 87, 1596-1605.	0.2	88
117	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
118	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
119	Computer Simulation of Incommensurate Diffusion in Zeolites:Â Understanding Window Effects. Journal of Physical Chemistry B, 2003, 107, 12138-12152.	1.2	83
120	Loading Dependence of the Diffusion Coefficient of Methane in Nanoporous Materials. Journal of Physical Chemistry B, 2006, 110, 22754-22772.	1.2	80
121	Bias free multiobjective active learning for materials design and discovery. Nature Communications, 2021, 12, 2312.	5.8	78
122	Simulation of Alkane Adsorption in the Aluminophosphate Molecular Sieve AlPO4â^'5. Journal of Physical Chemistry B, 1998, 102, 7183-7189.	1.2	77
123	Molecular simulations of mesoscopic bilayer phases. Physical Review E, 2003, 67, 060901.	0.8	76
124	Improved United-Atom Force Field for 1-Alkyl-3-methylimidazolium Chloride. Journal of Physical Chemistry B, 2010, 114, 4572-4582.	1.2	76
125	Optimizing nanoporous materials for gas storage. Physical Chemistry Chemical Physics, 2014, 16, 5499.	1.3	76
126	Molecular Simulation of the Effect of Cholesterol on Lipid-Mediated Protein-Protein Interactions. Biophysical Journal, 2010, 99, 3629-3638.	0.2	75

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127	The Influence of Non-framework Sodium Cations on the Adsorption of Alkanes in MFI- and MOR-Type Zeolites. Journal of Physical Chemistry B, 2002, 106, 10659-10667.	1.2	74
128	Distinguishing Metalâ€“Organic Frameworks. Crystal Growth and Design, 2018, 18, 1738-1747.	1.4	74
129	Theoretical Simulation of n-Alkane Cracking on Zeolites. Journal of Physical Chemistry C, 2010, 114, 10229-10239.	1.5	73
130	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
131	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
132	First-principles Hubbard U approach for small molecule binding in metal-organic frameworks. Journal of Chemical Physics, 2016, 144, 174104.	1.2	73
133	Enhanced Visible-Light-Driven Hydrogen Production through MOF/MOF Heterojunctions. ACS Applied Materials & Interfaces, 2021, 13, 14239-14247.	4.0	73
134	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
135	Capillary Phase Transitions ofn-Alkanes in a Carbon Nanotube. Nano Letters, 2004, 4, 241-244.	4.5	71
136	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
137	Evaluating Charge Equilibration Methods To Generate Electrostatic Fields in Nanoporous Materials. Journal of Chemical Theory and Computation, 2019, 15, 382-401.	2.3	70
138	In silico design and screening of hypothetical MOF-74 analogs and their experimental synthesis. Chemical Science, 2016, 7, 6263-6272.	3.7	69
139	Adsorption and Diffusion ofn-Hexane/2-Methylpentane Mixtures in Zeolite Silicalite:Â Experiments and Modeling. Journal of Physical Chemistry B, 2001, 105, 7690-7698.	1.2	68
140	Understanding the Window Effect in Zeolite Catalysis. Angewandte Chemie - International Edition, 2003, 42, 3624-3626.	7.2	68
141	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
142	Improving the Mechanical Stability of Metalâ€“Organic Frameworks Using Chemical Caryatids. ACS Central Science, 2018, 4, 832-839.	5.3	67
143	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
144	Effect of surfactant structure on interfacial properties. Europhysics Letters, 2003, 63, 902-907.	0.7	65

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145	Simulation of adsorption and diffusion of hydrocarbons in zeolites. Faraday Discussions, 1997, 106, 93-104.	1.6	64
146	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
147	Unexpected Diffusion Anisotropy of Carbon Dioxide in the Metalâ€“Organic Framework Zn‹sub›2‹/sub›(dobpdc). Journal of the American Chemical Society, 2018, 140, 1663-1673.	6.6	64
148	Charge Separation and Charge Carrier Mobility in Photocatalytic Metalâ€Organic Frameworks. Advanced Functional Materials, 2020, 30, 2003792.	7.8	64
149	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
150	Vapor-liquid equilibria of model alkanes. Journal of the American Chemical Society, 1993, 115, 6454-6455.	6.6	63
151	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
152	Comparison of mesoscopic phospholipidâ€“water models. Physical Chemistry Chemical Physics, 2004, 6, 4142-4151.	1.3	62
153	A New United Atom Force Field for Adsorption of Alkenes in Zeolites. Journal of Physical Chemistry C, 2008, 112, 2492-2498.	1.5	62
154	Simulating Tethered Polymer Layers in Shear Flow with the Dissipative Particle Dynamics Technique. Macromolecules, 2002, 35, 7138-7148.	2.2	61
155	Understanding cage effects in the n-alkane conversion on zeolites. Journal of Catalysis, 2006, 237, 278-290.	3.1	61
156	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
157	Separation of linear, mono-methyl and di-methyl alkanes in the 5â€“7 carbon atom range by exploiting configurational entropy effects during sorption on silicalite-1. Physical Chemistry Chemical Physics, 2001, 3, 4390-4398.	1.3	60
158	Shape selectivity through entropy. Journal of Catalysis, 2003, 214, 88-99.	3.1	60
159	Evaluation of various water models for simulation of adsorption in hydrophobic zeolites. Molecular Simulation, 2009, 35, 1067-1076.	0.9	60
160	In-Depth Study of the Influence of Hostâ^'Framework Flexibility on the Diffusion of Small Gas Molecules in One-Dimensional Zeolitic Pore Systems. Journal of Physical Chemistry C, 2007, 111, 17370-17381.	1.5	59
161	Combined Density Functional Theory and Monte Carlo Analysis of Monomolecular Cracking of Light Alkanes Over H-ZSM-5. Journal of Physical Chemistry C, 2012, 116, 23408-23417.	1.5	59
162	Commensurate Freezing ofn-Alkanes in Silicalite. Angewandte Chemie International Edition in English, 1995, 34, 2543-2544.	4.4	58

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163	Differences between MFI- and MEL-Type Zeolites in Paraffin Hydrocracking. Journal of Catalysis, 2001, 203, 281-291.	3.1	58
164	Nucleobase pairing and photodimerization in a biologically derived metal-organic framework nanoreactor. Nature Communications, 2019, 10, 1612.	5.8	58
165	A Molecular Mechanism of Hysteresis in Clay Swelling. Angewandte Chemie - International Edition, 2004, 43, 2650-2652.	7.2	57
166	High-Throughput Characterization of Porous Materials Using Graphics Processing Units. Journal of Chemical Theory and Computation, 2012, 8, 1684-1693.	2.3	57
167	Probing Adsorption Interactions in Metalâ€“Organic Frameworks using X-ray Spectroscopy. Journal of the American Chemical Society, 2013, 135, 18183-18190.	6.6	56
168	Pre-transition effects mediate forces of assembly between transmembrane proteins. ELife, 2016, 5, e13150.	2.8	56
169	Location and Conformation ofn-Alkanes in Zeolites:Â An Analysis of Configurational-Bias Monte Carlo Calculations. The Journal of Physical Chemistry, 1996, 100, 17573-17581.	2.9	54
170	Understanding Zeolite Catalysis: Inverse Shape Selectivity Revised. Angewandte Chemie - International Edition, 2002, 41, 2499-2502.	7.2	54
171	The Grand Challenges in Carbon Capture, Utilization, and Storage. Frontiers in Energy Research, 2014, 2, .	1.2	54
172	In Silico Discovery of High Deliverable Capacity Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2015, 119, 186-195.	1.5	54
173	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
174	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
175	Simulating the self-assembly of model membranes. PhysChemComm, 1999, 2, 45.	0.8	52
176	Molecular dynamics simulations of the surface tension of n-hexane, n-decane and n-hexadecane. Molecular Physics, 2002, 100, 2471-2475.	0.8	52
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