

Brian Space

List of Publications by Year in descending order

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168
papers

10,975
citations

38660

50
h-index

33814

99
g-index

175
all docs

175
docs citations

175
times ranked

7205
citing authors

#	ARTICLE	IF	CITATIONS
1	Porous materials with optimal adsorption thermodynamics and kinetics for CO ₂ separation. Nature, 2013, 495, 80-84.	13.7	2,005
2	Introduction of π -Complexation into Porous Aromatic Framework for Highly Selective Adsorption of Ethylene over Ethane. Journal of the American Chemical Society, 2014, 136, 8654-8660.	6.6	383
3	Robust Ultramicroporous Metal-Organic Frameworks with Benchmark Affinity for Acetylene. Angewandte Chemie - International Edition, 2018, 57, 10971-10975.	7.2	365
4	Synergistic sorbent separation for one-step ethylene purification from a four-component mixture. Science, 2019, 366, 241-246.	6.0	360
5	Benchmark C ₂ H ₂ /CO ₂ and CO ₂ /C ₂ H ₂ Separation by Two Closely Related Hybrid Ultramicroporous Materials. Chem, 2016, 1, 753-765.	5.8	349
6	A Stable Metal-Organic Framework Featuring a Local Buffer Environment for Carbon Dioxide Fixation. Angewandte Chemie - International Edition, 2018, 57, 4657-4662.	7.2	283
7	Tuning Pore Size in Square Lattice Coordination Networks for Size-Selective Sieving of CO ₂ . Angewandte Chemie - International Edition, 2016, 55, 10268-10272.	7.2	237
8	A Robust Molecular Porous Material with High CO ₂ Uptake and Selectivity. Journal of the American Chemical Society, 2013, 135, 10950-10953.	6.6	236
9	On the Mechanism of Hydrogen Storage in a Metal-Organic Framework Material. Journal of the American Chemical Society, 2007, 129, 15202-15210.	6.6	182
10	A Metal-Organic Framework Based Methane Nanotrap for the Capture of Coal-Mine Methane. Angewandte Chemie - International Edition, 2019, 58, 10138-10141.	7.2	181
11	A MOF-based Ultra-Strong Acetylene Nanotrap for Highly Efficient C ₂ H ₂ /H ₂ /CO ₂ Separation. Angewandte Chemie - International Edition, 2021, 60, 5283-5288.	7.2	172
12	Metal-Organic Framework Based Hydrogen-Bonding Nanotrap for Efficient Acetylene Storage and Separation. Journal of the American Chemical Society, 2022, 144, 1681-1689.	6.6	172
13	Reversible Switching between Highly Porous and Nonporous Phases of an Interpenetrated Diamondoid Coordination Network That Exhibits Gate-Opening at Methane Storage Pressures. Angewandte Chemie - International Edition, 2018, 57, 5684-5689.	7.2	161
14	Theoretical Modeling of Interface Specific Vibrational Spectroscopy: Methods and Applications to Aqueous Interfaces. Chemical Reviews, 2006, 106, 1234-1258.	23.0	159
15	Enhanced Gas Uptake in a Microporous Metal-Organic Framework via a Sorbate Induced-Fit Mechanism. Journal of the American Chemical Society, 2019, 141, 17703-17712.	6.6	152
16	Highly selective adsorption of ethylene over ethane in a MOF featuring the combination of open metal site and π -complexation. Chemical Communications, 2015, 51, 2714-2717.	2.2	151
17	Trace CO ₂ capture by an ultramicroporous physisorbent with low water affinity. Science Advances, 2019, 5, eaax9171.	4.7	143
18	Hybrid Ultra-Microporous Materials for Selective Xenon Adsorption and Separation. Angewandte Chemie - International Edition, 2016, 55, 8285-8289.	7.2	137

#	ARTICLE	IF	CITATIONS
19	Effect of ring rotation upon gas adsorption in SIFSIX-3-M (M = Fe, Ni) pillared square grid networks. <i>Chemical Science</i> , 2017, 8, 2373-2380.	3.7	121
20	Fine Tuning of MOF-505 Analogues To Reduce Low-Pressure Methane Uptake and Enhance Methane Working Capacity. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 11426-11430.	7.2	119
21	Nonadiabatic dynamics of excited excess electrons in simple fluids. <i>Journal of Chemical Physics</i> , 1991, 94, 1976-1984.	1.2	117
22	Highly Selective Separation of C ₂ H ₂ from CO ₂ by a New Dichromate-Based Hybrid Ultramicroporous Material. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 33395-33400.	4.0	116
23	Hydrophobic pillared square grids for selective removal of CO ₂ from simulated flue gas. <i>Chemical Communications</i> , 2015, 51, 15530-15533.	2.2	115
24	Highly Selective CO ₂ Uptake in Uninodal 6-Connected α -Nets Based upon MO ₄ ²⁺ (M = Cr, Mo) Pillars. <i>Journal of the American Chemical Society</i> , 2012, 134, 19556-19559.	6.6	110
25	Putting the Squeeze on CH ₄ and CO ₂ through Control over Interpenetration in Diamondoid Nets. <i>Journal of the American Chemical Society</i> , 2014, 136, 5072-5077.	6.6	106
26	A combined time correlation function and instantaneous normal mode study of the sum frequency generation spectroscopy of the water/vapor interface. <i>Journal of Chemical Physics</i> , 2003, 118, 8411-8419.	1.2	98
27	An Accurate and Transferable Intermolecular Diatomic Hydrogen Potential for Condensed Phase Simulation. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1332-1337.	2.3	91
28	Dynamics of trapping and localization of excess electrons in simple fluids. <i>Journal of Chemical Physics</i> , 1992, 96, 652-663.	1.2	87
29	Enhancement of CO ₂ selectivity in a pillared pcu MOM platform through pillar substitution. <i>Chemical Communications</i> , 2013, 49, 1606.	2.2	87
30	Robust Ultramicroporous Metal-Organic Frameworks with Benchmark Affinity for Acetylene. <i>Angewandte Chemie</i> , 2018, 130, 11137-11141.	1.6	85
31	Understanding the H ₂ Sorption Trends in the M-MOF-74 Series (M = Mg, Ni, Co, Zn). <i>Journal of Physical Chemistry C</i> , 2015, 119, 1078-1090.	1.5	84
32	A Molecular Dynamics Study of Aggregation Phenomena in Aqueous n-Propanol. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7389-7401.	1.2	81
33	Simulation of the Mechanism of Gas Sorption in a Metal-Organic Framework with Open Metal Sites: Molecular Hydrogen in PCN-61. <i>Journal of Physical Chemistry C</i> , 2012, 116, 15538-15549.	1.5	76
34	Understanding Hydrogen Sorption in a Metal-Organic Framework with Open-Metal Sites and Amide Functional Groups. <i>Journal of Physical Chemistry C</i> , 2013, 117, 9340-9354.	1.5	74
35	Characterization of Tunable Radical Metal-Carbenes: Key Intermediates in Catalytic Cyclopropanation. <i>Organometallics</i> , 2011, 30, 2739-2746.	1.1	73
36	Remote Stabilization of Copper Paddlewheel Based Molecular Building Blocks in Metal-Organic Frameworks. <i>Chemistry of Materials</i> , 2015, 27, 2144-2151.	3.2	72

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37	Halogenâ€C₂H₂ Binding in Ultramicroporous Metalâ€Organic Frameworks (MOFs) for Benchmark C₂H₂/CO₂ Separation Selectivity. Chemistry - A European Journal, 2020, 26, 4923-4929.	1.7	72
38	Atomic Charges Derived from Electrostatic Potentials for Molecular and Periodic Systems. Journal of Physical Chemistry A, 2010, 114, 10225-10233.	1.1	70
39	Robust Microporous Metalâ€Organic Frameworks for Highly Efficient and Simultaneous Removal of Propyne and Propadiene from Propylene. Angewandte Chemie - International Edition, 2019, 58, 10209-10214.	7.2	69
40	A combined instantaneous normal mode and time correlation function description of the infrared vibrational spectrum of ambient water. Journal of Chemical Physics, 1999, 111, 10622-10632.	1.2	68
41	Breaking the trade-off between selectivity and adsorption capacity for gas separation. Chem, 2021, 7, 3085-3098.	5.8	68
42	Crystal engineering of a family of hybrid ultramicroporous materials based upon interpenetration and dichromate linkers. Chemical Science, 2016, 7, 5470-5476.	3.7	66
43	One-step ethylene production from a four-component gas mixture by a single physisorbent. Nature Communications, 2021, 12, 6507.	5.8	64
44	The effect of isotopic substitution and detailed balance on the infrared spectroscopy of water: A combined time correlation function and instantaneous normal mode analysis. Journal of Chemical Physics, 2000, 112, 8083-8088.	1.2	63
45	Readily accessible shape-memory effect in a porous interpenetrated coordination network. Science Advances, 2018, 4, eaaq1636.	4.7	61
46	Aminoâ€Functionalised Hybrid Ultramicroporous Materials that Enable Singleâ€Step Ethylene Purification from a Ternary Mixture. Angewandte Chemie - International Edition, 2021, 60, 10902-10909.	7.2	56
47	Benchmark Acetylene Binding Affinity and Separation through Induced Fit in a Flexible Hybrid Ultramicroporous Material. Angewandte Chemie - International Edition, 2021, 60, 20383-20390.	7.2	56
48	A theoretical description of the polarization dependence of the sum frequency generation spectroscopy of the water/vapor interface. Journal of Chemical Physics, 2005, 123, 144705.	1.2	55
49	Simulations of hydrogen sorption in rht-MOF-1: identifying the binding sites through explicit polarization and quantum rotation calculations. Journal of Materials Chemistry A, 2014, 2, 2088-2100.	5.2	55
50	Radiation-resistant metal-organic framework enables efficient separation of krypton fission gas from spent nuclear fuel. Nature Communications, 2020, 11, 3103.	5.8	54
51	Efficient CO₂ Removal for Ultraâ€Pure CO Production by Two Hybrid Ultramicroporous Materials. Angewandte Chemie - International Edition, 2018, 57, 3332-3336.	7.2	52
52	Towards an understanding of the propensity for crystalline hydrate formation by molecular compounds. IUCr, 2016, 3, 430-439.	1.0	49
53	A MOFâ€based Ultraâ€Strong Acetylene Nanoâ€trap for Highly Efficient C₂H₂/CO₂ Separation. Angewandte Chemie, 2021, 133, 5343-5348.	1.6	49
54	The local electric field favours more than exposed nitrogen atoms on CO₂ capture: a case study on the rht-type MOF platform. Chemical Communications, 2015, 51, 9636-9639.	2.2	48

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55	Pillar substitution modulates CO ₂ affinity in μ MOF topology networks. <i>Chemical Communications</i> , 2013, 49, 9809.	2.2	47
56	Novel mode of 2-fold interpenetration observed in a primitive cubic network of formula [Ni(1,2-bis(4-pyridyl)acetylene) ₂ (Cr ₂ O ₇)] _n . <i>Chemical Communications</i> , 2015, 51, 14832-14835.	2.2	47
57	Self-Adjusting Metal-Organic Framework for Efficient Capture of Trace Xenon and Krypton. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	47
58	Computational Studies of CO ₂ Sorption and Separation in an Ultramicroporous Metal-Organic Material. <i>Journal of Physical Chemistry C</i> , 2013, 117, 17687-17698.	1.5	45
59	New Reticular Chemistry of the Rod Secondary Building Unit: Synthesis, Structure, and Natural Gas Storage of a Series of Three-Way Rod Amide-Functionalized Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2021, 143, 12202-12211.	6.6	44
60	Hydrogen adsorbed in a metal organic framework-5: Coupled translation-rotation eigenstates from quantum five-dimensional calculations. <i>Journal of Chemical Physics</i> , 2012, 137, 014701.	1.2	43
61	Tuning Pore Size in Square Lattice Coordination Networks for Size-Selective Sieving of CO ₂ . <i>Angewandte Chemie</i> , 2016, 128, 10424-10428.	1.6	43
62	Vibrationally resolved shape resonant photoionization of N ₂ O. <i>Journal of Chemical Physics</i> , 1989, 90, 1544-1550.	1.2	42
63	Long time scale molecular dynamics subspace integration method applied to anharmonic crystals and glasses. <i>Journal of Chemical Physics</i> , 1993, 99, 9070-9079.	1.2	42
64	A Predictive Model of Hydrogen Sorption for Metal-Organic Materials. <i>Journal of Physical Chemistry C</i> , 2009, 113, 9316-9320.	1.5	41
65	Investigating the Gas Sorption Mechanism in an <i>ir</i> -Metal-Organic Framework through Computational Studies. <i>Journal of Physical Chemistry C</i> , 2014, 118, 439-456.	1.5	40
66	Capturing the H ₂ -Metal Interaction in Mg-MOF-74 Using Classical Polarization. <i>Journal of Physical Chemistry C</i> , 2014, 118, 22683-22690.	1.5	40
67	The effect of centred versus offset interpenetration on C ₂ H ₂ sorption in hybrid ultramicroporous materials. <i>Chemical Communications</i> , 2017, 53, 11592-11595.	2.2	40
68	A robust soc-MOF platform exhibiting high gravimetric uptake and volumetric deliverable capacity for on-board methane storage. <i>Nano Research</i> , 2021, 14, 512-517.	5.8	40
69	A Polarizable and Transferable PHAST CO ₂ Potential for Materials Simulation. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5421-5429.	2.3	39
70	A combined instantaneous normal mode and time correlation function description of the optical Kerr effect and Raman spectroscopy of liquid CS ₂ . <i>Journal of Chemical Physics</i> , 2000, 112, 4186-4192.	1.2	38
71	A time correlation function theory of two-dimensional infrared spectroscopy with applications to liquid water. <i>Journal of Chemical Physics</i> , 2004, 121, 3688-3701.	1.2	38
72	Hybrid Ultra-Microporous Materials for Selective Xenon Adsorption and Separation. <i>Angewandte Chemie</i> , 2016, 128, 8425-8429.	1.6	38

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73	Impact of partial interpenetration in a hybrid ultramicroporous material on C ₂ /H ₂ /C ₂ /H ₄ separation performance. Chemical Communications, 2018, 54, 3488-3491.	2.2	38
74	Identification of a wagging vibrational mode of water molecules at the water/vapor interface. Physical Review E, 2005, 71, 050601.	0.8	37
75	Theoretical Investigations of CO ₂ and H ₂ Sorption in an Interpenetrated Square-Pillared Metal-Organic Material. Journal of Physical Chemistry C, 2013, 117, 9970-9982.	1.5	36
76	Theoretical Investigations of CO ₂ and CH ₄ Sorption in an Interpenetrated Diamondoid Metal-Organic Material. Langmuir, 2014, 30, 6454-6462.	1.6	35
77	Investigating CO ₂ Sorption in SIFSIX-3-M (M = Fe, Co, Ni, Cu, Zn) through Computational Studies. Crystal Growth and Design, 2019, 19, 3732-3743.	1.4	35
78	Fine Tuning of MOF-505 Analogues To Reduce Low-Pressure Methane Uptake and Enhance Methane Working Capacity. Angewandte Chemie, 2017, 129, 11584-11588.	1.6	33
79	Efficient calculation of many-body induced electrostatics in molecular systems. Journal of Chemical Physics, 2013, 139, 184112.	1.2	32
80	Understanding Hydrogen Sorption in In-soc-MOF: A Charged Metal-Organic Framework with Open-Metal Sites, Narrow Channels, and Counterions. Crystal Growth and Design, 2015, 15, 1460-1471.	1.4	32
81	A Stable Metal-Organic Framework Featuring a Local Buffer Environment for Carbon Dioxide Fixation. Angewandte Chemie, 2018, 130, 4747-4752.	1.6	32
82	Highly selective CO ₂ removal for one-step liquefied natural gas processing by physisorbents. Chemical Communications, 2019, 55, 3219-3222.	2.2	31
83	A time correlation function theory for the fifth order Raman response function with applications to liquid CS ₂ . Journal of Chemical Physics, 2003, 119, 6073-6082.	1.2	30
84	Immobilization of a Polar Sulfone Moiety onto the Pore Surface of a Humid-Stable MOF for Highly Efficient CO ₂ Separation under Dry and Wet Environments through Direct CO ₂ -Sulfone Interactions. ACS Applied Materials & Interfaces, 2020, 12, 41177-41184.	4.0	30
85	An instantaneous normal mode theory of condensed phase absorption: The collision-induced absorption spectra of liquid CO ₂ . Journal of Chemical Physics, 1997, 107, 5635-5644.	1.2	29
86	Metal-organic materials with triazine-based ligands: From structures to properties and applications. Coordination Chemistry Reviews, 2021, 427, 213518.	9.5	29
87	A high rotational barrier for physisorbed hydrogen in an fcu-metal-organic framework. Chemical Communications, 2014, 50, 14109-14112.	2.2	28
88	A Metal-Organic Framework Based Methane Nano-trap for the Capture of Coal-Mine Methane. Angewandte Chemie, 2019, 131, 10244-10247.	1.6	28
89	Indium-Organic Framework with <i>soc</i> Topology as a Versatile Catalyst for Highly Efficient One-Pot Strecker Synthesis of α -aminonitriles. ACS Applied Materials & Interfaces, 2021, 13, 52023-52033.	4.0	28
90	Ultramicropore Engineering by Dehydration to Enable Molecular Sieving of H ₂ by Calcium Trimesate. Angewandte Chemie - International Edition, 2020, 59, 16188-16194.	7.2	28

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91	Dielectric analysis of poly(methyl methacrylate) zinc(II) mono-pinacolborane diphenylporphyrin composites. <i>Polymer</i> , 2010, 51, 4790-4805.	1.8	27
92	Dramatic effect of pore size reduction on the dynamics of hydrogen adsorbed in metal-organic materials. <i>Journal of Materials Chemistry A</i> , 2014, 2, 13884.	5.2	27
93	Reversible Switching between Highly Porous and Nonporous Phases of an Interpenetrated Diamondoid Coordination Network That Exhibits Gate-Opening at Methane Storage Pressures. <i>Angewandte Chemie</i> , 2018, 130, 5786-5791.	1.6	27
94	Investigating H ₂ Sorption in a Fluorinated Metal-Organic Framework with Small Pores Through Molecular Simulation and Inelastic Neutron Scattering. <i>Langmuir</i> , 2015, 31, 7328-7336.	1.6	26
95	Molecular Sieving and Direct Visualization of CO ₂ in Binding Pockets of an Ultramicroporous Lanthanide Metal-Organic Framework Platform. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 23192-23197.	4.0	26
96	Efficient propyne/propadiene separation by microporous crystalline physisorbents. <i>Nature Communications</i> , 2021, 12, 5768.	5.8	26
97	Exceptional H ₂ sorption characteristics in a Mg ²⁺ -based metal-organic framework with small pores: insights from experimental and theoretical studies. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1786-1796.	1.3	24
98	Predictive models of gas sorption in a metal-organic framework with open-metal sites and small pore sizes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 18587-18602.	1.3	24
99	A theoretical investigation of the temperature dependence of the optical Kerr effect and Raman spectroscopy of liquid CS ₂ . <i>Journal of Chemical Physics</i> , 2000, 113, 8693-8699.	1.2	23
100	Understanding hydrogen sorption in a polar metal-organic framework with constricted channels. <i>Journal of Chemical Physics</i> , 2012, 136, 034705.	1.2	23
101	Modeling PCN-61 and PCN-66: Isostructural <i>h</i> -Metal-Organic Frameworks with Distinct CO ₂ Sorption Mechanisms. <i>Crystal Growth and Design</i> , 2014, 14, 5599-5607.	1.4	23
102	Dynamics of H ₂ adsorbed in porous materials as revealed by computational analysis of inelastic neutron scattering spectra. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17141-17158.	1.3	23
103	Dramatic Effect of the Electrostatic Parameters on H ₂ Sorption in an M-MOF-74 Analogue. <i>Crystal Growth and Design</i> , 2016, 16, 867-874.	1.4	23
104	A Microporous Co-MOF for Highly Selective CO ₂ Sorption in High Loadings Involving Aryl C-H...O...C...O Interactions: Combined Simulation and Breakthrough Studies. <i>Inorganic Chemistry</i> , 2019, 58, 11553-11560.	1.9	23
105	Feasibility of using photophoresis to create a concentration gradient of solvated molecules. <i>Journal of Chemical Physics</i> , 1996, 105, 9515-9524.	1.2	22
106	Comparing the mechanism and energetics of CO ₂ sorption in the SIFSIX series. <i>CrystEngComm</i> , 2017, 19, 3338-3347.	1.3	22
107	A robust heterometallic ultramicroporous MOF with ultrahigh selectivity for propyne/propylene separation. <i>Journal of Materials Chemistry A</i> , 2021, 9, 2850-2856.	5.2	22
108	Vibrationally resolved electronic autoionization of core-hole resonances. <i>Journal of Chemical Physics</i> , 1988, 89, 4048-4053.	1.2	21

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109	Subspace Method for Long Time Scale Molecular Dynamics. <i>The Journal of Physical Chemistry</i> , 1995, 99, 7330-7338.	2.9	21
110	A molecular H ₂ potential for heterogeneous simulations including polarization and many-body van der Waals interactions. <i>Journal of Chemical Physics</i> , 2012, 136, 194302.	1.2	21
111	Crystal Engineering of a 4,6-c fsc Platform That Can Serve as a Carbon Dioxide Single-Molecule Trap. <i>Crystal Growth and Design</i> , 2016, 16, 1071-1080.	1.4	21
112	Experimental and theoretical investigations of the gas adsorption sites in rht-metal-organic frameworks. <i>CrystEngComm</i> , 2017, 19, 4646-4665.	1.3	20
113	An instantaneous normal mode theory of condensed phase absorption: the vibrational spectrum of condensed CS ₂ from boiling to freezing. <i>Chemical Physics Letters</i> , 1998, 296, 259-265.	1.2	18
114	Time correlation function and finite field approaches to the calculation of the fifth order Raman response in liquid xenon. <i>Journal of Chemical Physics</i> , 2006, 125, 234501.	1.2	18
115	Examining the Effects of Different Ring Configurations and Equatorial Fluorine Atom Positions on CO ₂ Sorption in [Cu(bpy) ₂ SiF ₆]. <i>Crystal Growth and Design</i> , 2013, 13, 4542-4548.	1.4	17
116	Accurate H ₂ Sorption Modeling in the rht-MOF NOTT-112 Using Explicit Polarization. <i>Crystal Growth and Design</i> , 2016, 16, 6024-6032.	1.4	17
117	Theoretical Investigations of CO ₂ and H ₂ Sorption in Robust Molecular Porous Materials. <i>Langmuir</i> , 2016, 32, 11492-11505.	1.6	17
118	The rotational dynamics of H ₂ adsorbed in covalent organic frameworks. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 13075-13082.	1.3	17
119	Hydrogen Adsorption in a Zeolitic Imidazolate Framework with lta Topology. <i>Journal of Physical Chemistry C</i> , 2018, 122, 15435-15445.	1.5	17
120	A Polarizable and Transferable PHAST N ₂ Potential for Use in Materials Simulation. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5550-5557.	2.3	16
121	Insights into an intriguing gas sorption mechanism in a polar metal-organic framework with open-metal sites and narrow channels. <i>Chemical Communications</i> , 2014, 50, 7283-7286.	2.2	16
122	Robust Microporous Metal-Organic Frameworks for Highly Efficient and Simultaneous Removal of Propyne and Propadiene from Propylene. <i>Angewandte Chemie</i> , 2019, 131, 10315-10320.	1.6	16
123	Insights into the Gas Adsorption Mechanisms in Metal-Organic Frameworks from Classical Molecular Simulations. <i>Topics in Current Chemistry</i> , 2020, 378, 14.	3.0	16
124	Evidence for Substrate Preorganization in the Peptidylglycine Î±-Amidating Monooxygenase Reaction Describing the Contribution of Ground State Structure to Hydrogen Tunneling. <i>Journal of the American Chemical Society</i> , 2010, 132, 16393-16402.	6.6	15
125	Simulations of hydrogen, carbon dioxide, and small hydrocarbon sorption in a nitrogen-rich rht-metal-organic framework. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 1761-1777.	1.3	15
126	A Molecular Dynamics Method for Calculating Molecular Volume Changes Appropriate for Biomolecular Simulation. <i>Biophysical Journal</i> , 2003, 85, 2801-2807.	0.2	14

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127	Theoretical Insights into the Tuning of Metal Binding Sites of Paddlewheels in μ -Metal-Organic Frameworks. <i>ChemPhysChem</i> , 2015, 16, 3170-3179.	1.0	14
128	Benchmark Acetylene Binding Affinity and Separation through Induced Fit in a Flexible Hybrid Ultramicroporous Material. <i>Angewandte Chemie</i> , 2021, 133, 20546-20553.	1.6	14
129	Interchannel interactions following shape resonant excitation of core electrons. <i>Chemical Physics</i> , 1989, 129, 65-71.	0.9	13
130	A Novel Technique for the Measurement of Polarization-Specific Ultrafast Raman Responses. <i>Journal of Physical Chemistry A</i> , 2001, 105, 9851-9858.	1.1	13
131	Theoretical Investigation of the Temperature Dependence of the Fifth-Order Raman Response Function of Fluid and Liquid Xenon. <i>Journal of Physical Chemistry B</i> , 2006, 110, 3773-3781.	1.2	13
132	High H_2 Sorption Energetics in Zeolitic Imidazolate Frameworks. <i>Journal of Physical Chemistry C</i> , 2017, 121, 1723-1733.	1.5	13
133	Toward an Understanding of the Propensity for Crystalline Hydrate Formation by Molecular Compounds. Part 2. <i>Crystal Growth and Design</i> , 2021, 21, 4927-4939.	1.4	13
134	Tractable theory of nonlinear response and multidimensional nonlinear spectroscopy. <i>Physical Review E</i> , 2004, 70, 050101.	0.8	12
135	Efficient CO_2 Removal for Ultra-Pure CO Production by Two Hybrid Ultramicroporous Materials. <i>Angewandte Chemie</i> , 2018, 130, 3390-3394.	1.6	12
136	Applications of a time correlation function theory for the fifth-order Raman response function I: Atomic liquids. <i>Journal of Chemical Physics</i> , 2005, 123, 194507.	1.2	11
137	Generalized Computational Time Correlation Function Approach: Quantifying Quadrupole Contributions to Vibrationally Resonant Second-Order Interface-Specific Optical Spectroscopies. <i>Journal of Physical Chemistry C</i> , 2007, 111, 8749-8756.	1.5	11
138	An unusual H_2 sorption mechanism in PCN-14: insights from molecular simulation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21421-21430.	1.3	11
139	Inelastic Neutron Scattering and Theoretical Studies of H_2 Sorption in a Dy(III)-Based Phosphine Coordination Material. <i>Chemistry of Materials</i> , 2015, 27, 7619-7626.	3.2	10
140	Amino-Functionalised Hybrid Ultramicroporous Materials that Enable Single-Step Ethylene Purification from a Ternary Mixture. <i>Angewandte Chemie</i> , 2021, 133, 10997-11004.	1.6	10
141	An atomically detailed description of metal-dielectric interfaces: The crossover from surface to bulk conducting properties of Ag - Xe . <i>Journal of Chemical Physics</i> , 2000, 112, 10998-11004.	1.2	9
142	Photophysical Studies of the Trans to Cis Isomerization of the Push-Pull Molecule: 1-(Pyridin-4-yl)-2-(<i>N</i> -methylpyrrol-2-yl)ethene (mepepy). <i>Journal of Physical Chemistry A</i> , 2008, 112, 8310-8315.	1.1	9
143	Investigating the Effects of Linker Extension on H_2 Sorption in the μ -Metal-Organic Framework NU-111 by Molecular Simulations. <i>Crystal Growth and Design</i> , 2018, 18, 7599-7610.	1.4	9
144	Tuning the Selectivity between C_2H_2 and CO_2 in Molecular Porous Materials. <i>Langmuir</i> , 2021, 37, 13838-13845.	1.6	9

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