

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	Self-Adjusting Metal-Organic Framework for Efficient Capture of Trace Xenon and Krypton. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	5
2	Self-Adjusting Metal-Organic Framework for Efficient Capture of Trace Xenon and Krypton. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	47
3	Investigating H ₂ Adsorption in Isostructural Metal-Organic Frameworks M-CUK-1 (M = Co) Tj ETQq1 1 0.784314 rgBT 14, 8126-8136.	4.0	5
4	Metal-Organic Framework Based Hydrogen-Bonding Nanotrap for Efficient Acetylene Storage and Separation. <i>Journal of the American Chemical Society</i> , 2022, 144, 1681-1689.	6.6	172
5	Methane storage in flexible and dynamical metal-organic frameworks. <i>Chemical Physics Reviews</i> , 2022, 3, .	2.6	7
6	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
7	Metal-organic materials with triazine-based ligands: From structures to properties and applications. <i>Coordination Chemistry Reviews</i> , 2021, 427, 213518.	9.5	29
8	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
9	A MOF-based Ultra-Strong Acetylene Nano-Trap for Highly Efficient C ₂ H ₂ /CO ₂ Separation. <i>Angewandte Chemie</i> , 2021, 133, 5343-5348.	1.6	49
10	Frontispiz: A MOF-based Ultra-Strong Acetylene Nano-Trap for Highly Efficient C ₂ H ₂ /CO ₂ Separation. <i>Angewandte Chemie</i> , 2021, 133, .	1.6	1
11	Frontispiece: A MOF-based Ultra-Strong Acetylene Nano-Trap for Highly Efficient C ₂ H ₂ /CO ₂ Separation. <i>Angewandte Chemie - International Edition</i> , 2021, 60, .	7.2	0
12	A MOF-based Ultra-Strong Acetylene Nano-Trap for Highly Efficient C ₂ H ₂ /CO ₂ Separation. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 5283-5288.	7.2	172
13	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
14	Amino-Functionalised Hybrid Ultramicroporous Materials that Enable Single-Step Ethylene Purification from a Ternary Mixture. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 10902-10909.	7.2	56
15	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
16	Indium-Organic Framework with <i>soc</i> Topology as a Versatile Catalyst for Highly Efficient One-Pot Strecker Synthesis of Î±-aminonitriles. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 52023-52033.	4.0	28
17	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
18	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

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19	Breaking the trade-off between selectivity and adsorption capacity for gas separation. <i>CheM</i> , 2021, 7, 3085-3098.	5.8	68
20	Benchmark Acetylene Binding Affinity and Separation through Induced Fit in a Flexible Hybrid Ultramicroporous Material. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 20383-20390.	7.2	56
21	Efficient propyne/propadiene separation by microporous crystalline physisorbents. <i>Nature Communications</i> , 2021, 12, 5768.	5.8	26
22	One-step ethylene production from a four-component gas mixture by a single physisorbent. <i>Nature Communications</i> , 2021, 12, 6507.	5.8	64
23	Tuning the Selectivity between C ₂ H ₂ and CO ₂ in Molecular Porous Materials. <i>Langmuir</i> , 2021, 37, 13838-13845.	1.6	9
24	Halogen- ² C ₂ H ₂ Binding in Ultramicroporous Metal-Organic Frameworks (MOFs) for Benchmark C ₂ H ₂ /CO ₂ Separation Selectivity. <i>Chemistry - A European Journal</i> , 2020, 26, 4923-4929.	1.7	72
25	Next-Generation Accurate, Transferable, and Polarizable Potentials for Material Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7632-7644.	2.3	5
26	Innentitelbild: Ultramicropore Engineering by Dehydration to Enable Molecular Sieving of H ₂ by Calcium Trimesate (<i>Angew. Chem.</i> 37/2020). <i>Angewandte Chemie</i> , 2020, 132, 15898-15898.	1.6	0
27	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. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 41177-41184.	4.0	30
28	Simulations of H ₂ Sorption in an Anthracene-Functionalized h -Metal-Organic Framework. <i>Journal of Physical Chemistry C</i> , 2020, 124, 13753-13764.	1.5	1
29	Radiation-resistant metal-organic framework enables efficient separation of krypton fission gas from spent nuclear fuel. <i>Nature Communications</i> , 2020, 11, 3103.	5.8	54
30	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
31	Ultramicropore Engineering by Dehydration to Enable Molecular Sieving of H ₂ by Calcium Trimesate. <i>Angewandte Chemie</i> , 2020, 132, 16322-16328.	1.6	8
32	Ultramicropore Engineering by Dehydration to Enable Molecular Sieving of H ₂ by Calcium Trimesate. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 16188-16194.	7.2	28
33	Insights into the Gas Adsorption Mechanisms in Metal-Organic Frameworks from Classical Molecular Simulations. <i>Topics in Current Chemistry Collections</i> , 2020, , 215-279.	0.2	2
34	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, 1911553-11560.		23
35	MPMC and MCMD: Free High-Performance Simulation Software for Atomistic Systems. <i>Advanced Theory and Simulations</i> , 2019, 2, 1900113.	1.3	8
36	Enhanced Gas Uptake in a Microporous Metal-Organic Framework <i>via</i> a Sorbate Induced-Fit Mechanism. <i>Journal of the American Chemical Society</i> , 2019, 141, 17703-17712.	6.6	152

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37	Synergistic sorbent separation for one-step ethylene purification from a four-component mixture. <i>Science</i> , 2019, 366, 241-246.	6.0	360
38	A Metal-Organic Framework Based Methane Nano-trap for the Capture of Coal-Mine Methane. <i>Angewandte Chemie</i> , 2019, 131, 10244-10247.	1.6	28
39	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
40	Investigating CO ₂ Sorption in SIFSIX-3-M (M = Fe, Co, Ni, Cu, Zn) through Computational Studies. <i>Crystal Growth and Design</i> , 2019, 19, 3732-3743.	1.4	35
41	A Metal-Organic Framework Based Methane Nano-trap for the Capture of Coal-Mine Methane. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 10138-10141.	7.2	181
42	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
43	Robust Microporous Metal-Organic Frameworks for Highly Efficient and Simultaneous Removal of Propyne and Propadiene from Propylene. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 10209-10214.	7.2	69
44	Highly selective CO ₂ removal for one-step liquefied natural gas processing by physisorbents. <i>Chemical Communications</i> , 2019, 55, 3219-3222.	2.2	31
45	Innenrücktitelbild: A Metal-Organic Framework Based Methane Nano-trap for the Capture of Coal-Mine Methane (<i>Angew. Chem.</i> 30/2019). <i>Angewandte Chemie</i> , 2019, 131, 10483-10483.	1.6	0
46	Trace CO ₂ capture by an ultramicroporous physisorbent with low water affinity. <i>Science Advances</i> , 2019, 5, eaax9171.	4.7	143
47	A Stable Metal-Organic Framework Featuring a Local Buffer Environment for Carbon Dioxide Fixation. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 4657-4662.	7.2	283
48	A Stable Metal-Organic Framework Featuring a Local Buffer Environment for Carbon Dioxide Fixation. <i>Angewandte Chemie</i> , 2018, 130, 4747-4752.	1.6	32
49	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 - International Edition</i> , 2018, 57, 5684-5689.	7.2	161
50	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
51	Efficient CO ₂ Removal for Ultra-pure CO Production by Two Hybrid Ultramicroporous Materials. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 3332-3336.	7.2	52
52	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
53	Simulations of hydrogen, carbon dioxide, and small hydrocarbon sorption in a nitrogen-rich metal-organic framework. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 1761-1777.	1.3	15
54	Readily accessible shape-memory effect in a porous interpenetrated coordination network. <i>Science Advances</i> , 2018, 4, eaaq1636.	4.7	61

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55	Impact of partial interpenetration in a hybrid ultramicroporous material on C_2H_2/C_2H_4 separation performance. Chemical Communications, 2018, 54, 3488-3491.	2.2	38
56	Investigating the Effects of Linker Extension on H_2 Sorption in the rht-Metal-Organic Framework NU-111 by Molecular Simulations. Crystal Growth and Design, 2018, 18, 7599-7610.	1.4	9
57	Robust Ultramicroporous Metal-Organic Frameworks with Benchmark Affinity for Acetylene. Angewandte Chemie, 2018, 130, 11137-11141.	1.6	85
58	Robust Ultramicroporous Metal-Organic Frameworks with Benchmark Affinity for Acetylene. Angewandte Chemie - International Edition, 2018, 57, 10971-10975.	7.2	365
59	Investigating C_2H_2 Sorption in $[M_3(O_2CH)_6]$ (M = Mg, Mn) Through Theoretical Studies. Crystal Growth and Design, 2018, 18, 5342-5352.	1.4	2
60	Hydrogen Adsorption in a Zeolitic Imidazolate Framework with Ita Topology. Journal of Physical Chemistry C, 2018, 122, 15435-15445.	1.5	17
61	Theoretical study of the effect of halogen substitution in molecular porous materials for CO_2 and C_2H_2 sorption. AIMS Materials Science, 2018, 5, 226-245.	0.7	1
62	Highly Selective Separation of C_2H_2 from CO_2 by a New Dichromate-Based Hybrid Ultramicroporous Material. ACS Applied Materials & Interfaces, 2017, 9, 33395-33400.	4.0	116
63	The rotational dynamics of H_2 adsorbed in covalent organic frameworks. Physical Chemistry Chemical Physics, 2017, 19, 13075-13082.	1.3	17
64	Predictive models of gas sorption in a metal-organic framework with open-metal sites and small pore sizes. Physical Chemistry Chemical Physics, 2017, 19, 18587-18602.	1.3	24
65	Comparing the mechanism and energetics of CO_2 sorption in the SIFSIX series. CrystEngComm, 2017, 19, 3338-3347.	1.3	22
66	High H_2 Sorption Energetics in Zeolitic Imidazolate Frameworks. Journal of Physical Chemistry C, 2017, 121, 1723-1733.	1.5	13
67	Effect of ring rotation upon gas adsorption in SIFSIX-3-M (M = Fe, Ni) pillared square grid networks. Chemical Science, 2017, 8, 2373-2380.	3.7	121
68	The effect of centred versus offset interpenetration on C_2H_2 sorption in hybrid ultramicroporous materials. Chemical Communications, 2017, 53, 11592-11595.	2.2	40
69	Investigating gas sorption in an rht-metal-organic framework with 1,2,3-triazole groups. Physical Chemistry Chemical Physics, 2017, 19, 29204-29221.	1.3	8
70	Experimental and theoretical investigations of the gas adsorption sites in rht-metal-organic frameworks. CrystEngComm, 2017, 19, 4646-4665.	1.3	20
71	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
72	Fine Tuning of MOF-505 Analogues To Reduce Low-Pressure Methane Uptake and Enhance Methane Working Capacity. Angewandte Chemie - International Edition, 2017, 56, 11426-11430.	7.2	119

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73	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
74	Hybrid Ultra- μ Microporous Materials for Selective Xenon Adsorption and Separation. <i>Angewandte Chemie</i> , 2016, 128, 8425-8429.	1.6	38
75	Hybrid Ultra- μ Microporous Materials for Selective Xenon Adsorption and Separation. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 8285-8289.	7.2	137
76	Benchmark C ₂ H ₂ /CO ₂ and CO ₂ /C ₂ H ₂ Separation by Two Closely Related Hybrid Ultramicroporous Materials. <i>Chem</i> , 2016, 1, 753-765.	5.8	349
77	Towards an understanding of the propensity for crystalline hydrate formation by molecular compounds. <i>IUCr</i> , 2016, 3, 430-439.	1.0	49
78	Crystal engineering of a family of hybrid ultramicroporous materials based upon interpenetration and dichromate linkers. <i>Chemical Science</i> , 2016, 7, 5470-5476.	3.7	66
79	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
80	Accurate H ₂ Sorption Modeling in the <i>irht</i> -MOF NOTT-112 Using Explicit Polarization. <i>Crystal Growth and Design</i> , 2016, 16, 6024-6032.	1.4	17
81	Tuning Pore Size in Square- μ Lattice Coordination Networks for Size- μ Selective Sieving of CO ₂ . <i>Angewandte Chemie</i> , 2016, 128, 10424-10428.	1.6	43
82	Tuning Pore Size in Square- μ Lattice Coordination Networks for Size- μ Selective Sieving of CO ₂ . <i>Angewandte Chemie - International Edition</i> , 2016, 55, 10268-10272.	7.2	237
83	Theoretical Investigations of CO ₂ and H ₂ Sorption in Robust Molecular Porous Materials. <i>Langmuir</i> , 2016, 32, 11492-11505.	1.6	17
84	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
85	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
86	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
87	Theoretical Insights into the Tuning of Metal Binding Sites of Paddlewheels in <i>irht</i> -Metal-Organic Frameworks. <i>ChemPhysChem</i> , 2015, 16, 3170-3179.	1.0	14
88	Understanding Hydrogen Sorption in In- <i>soc</i> -MOF: A Charged Metal-Organic Framework with Open-Metal Sites, Narrow Channels, and Counterions. <i>Crystal Growth and Design</i> , 2015, 15, 1460-1471.	1.4	32
89	Highly selective adsorption of ethylene over ethane in a MOF featuring the combination of open metal site and π -complexation. <i>Chemical Communications</i> , 2015, 51, 2714-2717.	2.2	151
90	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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91	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
92	The local electric field favours more than exposed nitrogen atoms on CO ₂ capture: a case study on the <i>rht</i> -type MOF platform. <i>Chemical Communications</i> , 2015, 51, 9636-9639.	2.2	48
93	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
94	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
95	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
96	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
97	Time Correlation Function Modeling of Third-Order Sum Frequency Vibrational Spectroscopy of a Charged Surface/Water Interface. <i>Journal of Physical Chemistry B</i> , 2015, 119, 9219-9224.	1.2	5
98	Investigating the Gas Sorption Mechanism in an <i>rht</i> -Metal-Organic Framework through Computational Studies. <i>Journal of Physical Chemistry C</i> , 2014, 118, 439-456.	1.5	40
99	Modeling PCN-61 and PCN-66: Isostructural <i>rht</i> -Metal-Organic Frameworks with Distinct CO ₂ Sorption Mechanisms. <i>Crystal Growth and Design</i> , 2014, 14, 5599-5607.	1.4	23
100	A high rotational barrier for physisorbed hydrogen in an <i>fcu</i> -metal-organic framework. <i>Chemical Communications</i> , 2014, 50, 14109-14112.	2.2	28
101	Simulations of hydrogen sorption in <i>rht</i> -MOF-1: identifying the binding sites through explicit polarization and quantum rotation calculations. <i>Journal of Materials Chemistry A</i> , 2014, 2, 2088-2100.	5.2	55
102	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
103	Theoretical Investigations of CO ₂ and CH ₄ Sorption in an Interpenetrated Diamondoid Metal-Organic Material. <i>Langmuir</i> , 2014, 30, 6454-6462.	1.6	35
104	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
105	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
106	Introduction of π -Complexation into Porous Aromatic Framework for Highly Selective Adsorption of Ethylene over Ethane. <i>Journal of the American Chemical Society</i> , 2014, 136, 8654-8660.	6.6	383
107	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
108	A Robust Molecular Porous Material with High CO ₂ Uptake and Selectivity. <i>Journal of the American Chemical Society</i> , 2013, 135, 10950-10953.	6.6	236

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109	Pillar substitution modulates CO ₂ affinity in μ -topology networks. <i>Chemical Communications</i> , 2013, 49, 9809.	2.2	47
110	Enhancement of CO ₂ selectivity in a pillared pcu MOM platform through pillar substitution. <i>Chemical Communications</i> , 2013, 49, 1606.	2.2	87
111	Porous materials with optimal adsorption thermodynamics and kinetics for CO ₂ separation. <i>Nature</i> , 2013, 495, 80-84.	13.7	2,005
112	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
113	Theoretical Investigations of CO ₂ and H ₂ Sorption in an Interpenetrated Square-Pillared Metal-Organic Material. <i>Journal of Physical Chemistry C</i> , 2013, 117, 9970-9982.	1.5	36
114	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
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	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
117	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
118	Efficient calculation of many-body induced electrostatics in molecular systems. <i>Journal of Chemical Physics</i> , 2013, 139, 184112.	1.2	32
119	Solving the Many-Body Polarization Problem on GPUs: Application to MOFs. <i>Journal of Computational Science Education</i> , 2013, 4, 30-34.	0.3	2
120	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
121	A theoretical study of the sum frequency vibrational spectroscopy of the carbon tetrachloride/water interface. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 124108.	0.7	3
122	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
123	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
124	Highly Selective CO ₂ Uptake in Uninodal 6-Connected μ -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
125	Understanding hydrogen sorption in a polar metal-organic framework with constricted channels. <i>Journal of Chemical Physics</i> , 2012, 136, 034705.	1.2	23
126	Characterization of Tunable Radical Metal-Carbenes: Key Intermediates in Catalytic Cyclopropanation. <i>Organometallics</i> , 2011, 30, 2739-2746.	1.1	73

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127	Dielectric analysis of poly(methyl methacrylate) zinc(II) mono-pinacolborane diphenylporphyrin composites. <i>Polymer</i> , 2010, 51, 4790-4805.	1.8	27
128	Evidence for Substrate Preorganization in the Peptidylglycine β -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
129	Atomic Charges Derived from Electrostatic Potentials for Molecular and Periodic Systems. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10225-10233.	1.1	70
130	A Predictive Model of Hydrogen Sorption for Metal-Organic Materials. <i>Journal of Physical Chemistry C</i> , 2009, 113, 9316-9320.	1.5	41
131	Making a life in the physical sciences. <i>Journal of Organizational Behavior</i> , 2008, 29, 755-759.	2.9	1
132	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
133	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
134	On the Mechanism of Hydrogen Storage in a Metal-Organic Framework Material. <i>Journal of the American Chemical Society</i> , 2007, 129, 15202-15210.	6.6	182
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136	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
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