Brian Space

List of Publications by Year
in descending order

168 papers	10,975 citations	44444 50 h-index	38517 99 g-index
175 all docs	175 docs citations	175 times ranked	8210 citing authors

#	Article	IF	Citations
1	Selfâ€Adjusting Metalâ€“Organic Framework for Efficient Capture of Trace Xenon and Krypton. Angewandte Chemie, 2022, 134, .	1.6	5
2	Selfâ€Adjusting Metalâ€“Organic Framework for Efficient Capture of Trace Xenon and Krypton. Angewandte Chemie - International Edition, 2022, 61, .	7.2	47
3	Investigating H₂ Adsorption in Isostructural Metalâ€“Organic Frameworks M-CUK-1 (M = Co) Tj ETQq1 1 0.784314 rgBT /O 14, 8126-8136.	4.0	5
4	Metalâ€“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
5	Methane storage in flexible and dynamical metalâ€“organic frameworks. Chemical Physics Reviews, 2022, 3, .	2.6	7
6	A robust soc-MOF platform exhibiting high gravimetric uptake and volumetric deliverable capacity for on-board methane storage. Nano Research, 2021, 14, 512-517.	5.8	40
7	Metal-organic materials with triazine-based ligands: From structures to properties and applications. Coordination Chemistry Reviews, 2021, 427, 213518.	9.5	29
8	A robust heterometallic ultramicroporous MOF with ultrahigh selectivity for propyne/propylene separation. Journal of Materials Chemistry A, 2021, 9, 2850-2856.	5.2	22
9	A MOFâ€based Ultraâ€Strong Acetylene Nanoâ€trap for Highly Efficient C₂H₂/CO₂ Separation. Angewandte Chemie, 2021, 133, 5343-5348.	1.6	49
10	Frontispiz: A MOFâ€based Ultraâ€Strong Acetylene Nanoâ€trap for Highly Efficient C₂H₂/CO₂ Separation. Angewandte Chemie, 2021, 133, .	1.6	1
11	Frontispiece: A MOFâ€based Ultraâ€Strong Acetylene Nanoâ€trap for Highly Efficient C₂H₂/CO₂ Separation. Angewandte Chemie - International Edition, 2021, 60, .	7.2	0
12	A MOFâ€based Ultraâ€Strong Acetylene Nanoâ€trap for Highly Efficient C₂H₂/CO₂ Separation. Angewandte Chemie - International Edition, 2021, 60, 5283-5288.	7.2	172
13	Aminoâ€Functionalised Hybrid Ultramicroporous Materials that Enable Singleâ€Step Ethylene Purification from a Ternary Mixture. Angewandte Chemie, 2021, 133, 10997-11004.	1.6	10
14	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
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 Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2021, 143, 12202-12211.	6.6	44
16	Indiumâ€“Organic Framework with <i>soc</i> Topology as a Versatile Catalyst for Highly Efficient One-Pot Strecker Synthesis of Î±-aminonitriles. ACS Applied Materials & Interfaces, 2021, 13, 52023-52033.	4.0	28
17	Toward an Understanding of the Propensity for Crystalline Hydrate Formation by Molecular Compounds. Part 2. Crystal Growth and Design, 2021, 21, 4927-4939.	1.4	13
18	Benchmark Acetylene Binding Affinity and Separation through Induced Fit in a Flexible Hybrid Ultramicroporous Material. Angewandte Chemie, 2021, 133, 20546-20553.	1.6	14

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19	Breaking the trade-off between selectivity and adsorption capacity for gas separation. CheM, 2021, 7, 3085-3098.	5.8	68
20	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
21	Efficient propyne/propadiene separation by microporous crystalline physiadsorbents. Nature Communications, 2021, 12, 5768.	5.8	26
22	One-step ethylene production from a four-component gas mixture by a single physisorbent. Nature Communications, 2021, 12, 6507.	5.8	64
23	Tuning the Selectivity between C2H2 and CO2 in Molecular Porous Materials. Langmuir, 2021, 37, 13838-13845.	1.6	9
24	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
25	Next-Generation Accurate, Transferable, and Polarizable Potentials for Material Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7632-7644.	2.3	5
26	Innentitelbild: Ultramicropore Engineering by Dehydration to Enable Molecular Sieving of H₂ by Calcium Trimesate (Angew. Chem. 37/2020). Angewandte Chemie, 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 CO₂ Separation under Dry and Wet Environments through Direct CO₂â€“Sulfone Interactions. ACS Applied Materials & Interfaces, 2020, 12, 41177-41184.	4.0	30
28	Simulations of H₂ Sorption in an Anthracene-Functionalized rht-Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2020, 124, 13753-13764.	1.5	1
29	Radiation-resistant metal-organic framework enables efficient separation of krypton fission gas from spent nuclear fuel. Nature Communications, 2020, 11, 3103.	5.8	54
30	Insights into the Gas Adsorption Mechanisms in Metalâ€“Organic Frameworks from Classical Molecular Simulations. Topics in Current Chemistry, 2020, 378, 14.	3.0	16
31	Ultramicropore Engineering by Dehydration to Enable Molecular Sieving of H 2 by Calcium Trimesate. Angewandte Chemie, 2020, 132, 16322-16328.	1.6	8
32	Ultramicropore Engineering by Dehydration to Enable Molecular Sieving of H₂ by Calcium Trimesate. Angewandte Chemie - International Edition, 2020, 59, 16188-16194.	7.2	28
33	Insights into the Gas Adsorption Mechanisms in Metalâ€“Organic Frameworks from Classical Molecular Simulations. Topics in Current Chemistry Collections, 2020, , 215-279.	0.2	2
34	A Microporous Co-MOF for Highly Selective CO₂ Sorption in High Loadings Involving Aryl Câ€“HÂ·Â·Â·Oâ•Câ•O Interactions: Combined Simulation and Breakthrough Studies. Inorganic Chemistry, 2019, 58, 11553-11560.	1.9	23
35	MPMC and MCMD: Free Highâ€Performance Simulation Software for Atomistic Systems. Advanced Theory and Simulations, 2019, 2, 1900113.	1.3	8
36	Enhanced Gas Uptake in a Microporous Metalâ€“Organic Framework <i>via</i> a Sorbate Induced-Fit Mechanism. Journal of the American Chemical Society, 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. Science, 2019, 366, 241-246.	6.0	360
38	A Metalâ€“Organic Framework Based Methane Nanoâ€trap for the Capture of Coalâ€Mine Methane. Angewandte Chemie, 2019, 131, 10244-10247.	1.6	28
39	Molecular Sieving and Direct Visualization of CO₂ in Binding Pockets of an Ultramicroporous Lanthanide Metalâ€“Organic Framework Platform. ACS Applied Materials & Interfaces, 2019, 11, 23192-23197.	4.0	26
40	Investigating CO₂ 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
41	A Metalâ€“Organic Framework Based Methane Nanoâ€trap for the Capture of Coalâ€Mine Methane. Angewandte Chemie - International Edition, 2019, 58, 10138-10141.	7.2	181
42	Robust Microporous Metalâ€“Organic Frameworks for Highly Efficient and Simultaneous Removal of Propyne and Propadiene from Propylene. Angewandte Chemie, 2019, 131, 10315-10320.	1.6	16
43	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
44	Highly selective CO₂ removal for one-step liquefied natural gas processing by physisorbents. Chemical Communications, 2019, 55, 3219-3222.	2.2	31
45	InnenrÃ¼cktitelbild: A Metalâ€“Organic Framework Based Methane Nanoâ€trap for the Capture of Coalâ€Mine Methane (Angew. Chem. 30/2019). Angewandte Chemie, 2019, 131, 10483-10483.	1.6	0
46	Trace CO ₂ capture by an ultramicroporous physisorbent with low water affinity. Science Advances, 2019, 5, eaax9171.	4.7	143
47	A Stable Metalâ€“Organic Framework Featuring a Local Buffer Environment for Carbon Dioxide Fixation. Angewandte Chemie - International Edition, 2018, 57, 4657-4662.	7.2	283
48	A Stable Metalâ€“Organic Framework Featuring a Local Buffer Environment for Carbon Dioxide Fixation. Angewandte Chemie, 2018, 130, 4747-4752.	1.6	32
49	Reversible Switching between Highly Porous and Nonporous Phases of an Interpenetrated Diamondoid Coordination Network That Exhibits Gateâ€Opening at Methane Storage Pressures. Angewandte Chemie - International Edition, 2018, 57, 5684-5689.	7.2	161
50	Reversible Switching between Highly Porous and Nonporous Phases of an Interpenetrated Diamondoid Coordination Network That Exhibits Gateâ€Opening at Methane Storage Pressures. Angewandte Chemie, 2018, 130, 5786-5791.	1.6	27
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	Efficient CO₂ Removal for Ultraâ€Pure CO Production by Two Hybrid Ultramicroporous Materials. Angewandte Chemie, 2018, 130, 3390-3394.	1.6	12
53	Simulations of hydrogen, carbon dioxide, and small hydrocarbon sorption in a nitrogen-rich <i>rht</i>-metalâ€“organic framework. Physical Chemistry Chemical Physics, 2018, 20, 1761-1777.	1.3	15
54	Readily accessible shape-memory effect in a porous interpenetrated coordination network. Science Advances, 2018, 4, eaaq1636.	4.7	61

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55	Impact of partial interpenetration in a hybrid ultramicroporous material on C₂H₂/C₂H₄ separation performance. Chemical Communications, 2018, 54, 3488-3491.	2.2	38
56	Investigating the Effects of Linker Extension on H₂ Sorption in the rht-Metalâ€“Organic Framework NU-111 by Molecular Simulations. Crystal Growth and Design, 2018, 18, 7599-7610.	1.4	9
57	Robust Ultramicroporous Metalâ€“Organic Frameworks with Benchmark Affinity for Acetylene. Angewandte Chemie, 2018, 130, 11137-11141.	1.6	85
58	Robust Ultramicroporous Metalâ€“Organic Frameworks with Benchmark Affinity for Acetylene. Angewandte Chemie - International Edition, 2018, 57, 10971-10975.	7.2	365
59	Investigating C₂H₂ Sorption in Î±-[M₃(O₂CH)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 lta 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 CO₂ and C₂H₂ sorption. AIMS Materials Science, 2018, 5, 226-245.	0.7	1
62	Highly Selective Separation of C₂H₂ from CO₂ by a New Dichromate-Based Hybrid Ultramicroporous Material. ACS Applied Materials & Interfaces, 2017, 9, 33395-33400.	4.0	116
63	The rotational dynamics of H₂ adsorbed in covalent organic frameworks. Physical Chemistry Chemical Physics, 2017, 19, 13075-13082.	1.3	17
64	Predictive models of gas sorption in a metalâ€“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 CO₂ sorption in the SIFSIX series. CrystEngComm, 2017, 19, 3338-3347.	1.3	22
66	High H₂ 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 C₂H₂ sorption in hybrid ultramicroporous materials. Chemical Communications, 2017, 53, 11592-11595.	2.2	40
69	Investigating gas sorption in an rht-metalâ€“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-metalâ€“organic frameworks. CrystEngComm, 2017, 19, 4646-4665.	1.3	20
71	Fine Tuning of MOFâ€505 Analogues To Reduce Lowâ€Pressure Methane Uptake and Enhance Methane Working Capacity. Angewandte Chemie, 2017, 129, 11584-11588.	1.6	33
72	Fine Tuning of MOFâ€505 Analogues To Reduce Lowâ€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 H2 sorption mechanism in PCN-14: insights from molecular simulation. Physical Chemistry Chemical Physics, 2016, 18, 21421-21430.	1.3	11
74	Hybrid Ultraâ€Microporous Materials for Selective Xenon Adsorption and Separation. Angewandte Chemie, 2016, 128, 8425-8429.	1.6	38
75	Hybrid Ultraâ€Microporous Materials for Selective Xenon Adsorption and Separation. Angewandte Chemie - International Edition, 2016, 55, 8285-8289.	7.2	137
76	Benchmark C2H2/CO2 and CO2/C2H2 Separation by Two Closely Related Hybrid Ultramicroporous Materials. CheM, 2016, 1, 753-765.	5.8	349
77	Towards an understanding of the propensity for crystalline hydrate formation by molecular compounds. IUCrJ, 2016, 3, 430-439.	1.0	49
78	Crystal engineering of a family of hybrid ultramicroporous materials based upon interpenetration and dichromate linkers. Chemical Science, 2016, 7, 5470-5476.	3.7	66
79	Dynamics of H2 adsorbed in porous materials as revealed by computational analysis of inelastic neutron scattering spectra. Physical Chemistry Chemical Physics, 2016, 18, 17141-17158.	1.3	23
80	Accurate H₂ Sorption Modeling in the <i>rht</i>-MOF NOTT-112 Using Explicit Polarization. Crystal Growth and Design, 2016, 16, 6024-6032.	1.4	17
81	Tuning Pore Size in Squareâ€Lattice Coordination Networks for Sizeâ€Selective Sieving of CO₂. Angewandte Chemie, 2016, 128, 10424-10428.	1.6	43
82	Tuning Pore Size in Squareâ€Lattice Coordination Networks for Sizeâ€Selective Sieving of CO₂. Angewandte Chemie - International Edition, 2016, 55, 10268-10272.	7.2	237
83	Theoretical Investigations of CO₂ and H₂ Sorption in Robust Molecular Porous Materials. Langmuir, 2016, 32, 11492-11505.	1.6	17
84	Dramatic Effect of the Electrostatic Parameters on H2 Sorption in an M-MOF-74 Analogue. Crystal Growth and Design, 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. Crystal Growth and Design, 2016, 16, 1071-1080.	1.4	21
86	Exceptional H₂ sorption characteristics in a Mg²⁺-based metalâ€“organic framework with small pores: insights from experimental and theoretical studies. Physical Chemistry Chemical Physics, 2016, 18, 1786-1796.	1.3	24
87	Theoretical Insights into the Tuning of Metal Binding Sites of Paddlewheels in <i>rht</i>â€Metalâ€“Organic Frameworks. ChemPhysChem, 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. Crystal Growth and Design, 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 Ï€-complexation. Chemical Communications, 2015, 51, 2714-2717.	2.2	151
90	Remote Stabilization of Copper Paddlewheel Based Molecular Building Blocks in Metalâ€“Organic Frameworks. Chemistry of Materials, 2015, 27, 2144-2151.	3.2	72

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91	Investigating H2Sorption in a Fluorinated Metalâ€“Organic Framework with Small Pores Through Molecular Simulation and Inelastic Neutron Scattering. Langmuir, 2015, 31, 7328-7336.	1.6	26
92	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
93	Inelastic Neutron Scattering and Theoretical Studies of H2Sorption in a Dy(III)-Based Phosphine Coordination Material. Chemistry of Materials, 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(Cr₂O₇)]_n. Chemical Communications, 2015, 51, 14832-14835.	2.2	47
95	Hydrophobic pillared square grids for selective removal of CO₂ from simulated flue gas. Chemical Communications, 2015, 51, 15530-15533.	2.2	115
96	Understanding the H₂ Sorption Trends in the M-MOF-74 Series (M = Mg, Ni, Co, Zn). Journal of Physical Chemistry C, 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. Journal of Physical Chemistry B, 2015, 119, 9219-9224.	1.2	5
98	Investigating the Gas Sorption Mechanism in an <i>rht</i>-Metalâ€“Organic Framework through Computational Studies. Journal of Physical Chemistry C, 2014, 118, 439-456.	1.5	40
99	Modeling PCN-61 and PCN-66: Isostructural <i>rht</i>-Metalâ€“Organic Frameworks with Distinct CO₂ Sorption Mechanisms. Crystal Growth and Design, 2014, 14, 5599-5607.	1.4	23
100	A high rotational barrier for physisorbed hydrogen in an fcu-metalâ€“organic framework. Chemical Communications, 2014, 50, 14109-14112.	2.2	28
101	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
102	Dramatic effect of pore size reduction on the dynamics of hydrogen adsorbed in metalâ€“organic materials. Journal of Materials Chemistry A, 2014, 2, 13884.	5.2	27
103	Theoretical Investigations of CO₂ and CH₄ Sorption in an Interpenetrated Diamondoid Metalâ€“Organic Material. Langmuir, 2014, 30, 6454-6462.	1.6	35
104	Capturing the H₂â€“Metal Interaction in Mg-MOF-74 Using Classical Polarization. Journal of Physical Chemistry C, 2014, 118, 22683-22690.	1.5	40
105	Insights into an intriguing gas sorption mechanism in a polar metalâ€“organic framework with open-metal sites and narrow channels. Chemical Communications, 2014, 50, 7283-7286.	2.2	16
106	Introduction of Ï€-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
107	Putting the Squeeze on CH₄ and CO₂ through Control over Interpenetration in Diamondoid Nets. Journal of the American Chemical Society, 2014, 136, 5072-5077.	6.6	106
108	A Robust Molecular Porous Material with High CO₂ Uptake and Selectivity. Journal of the American Chemical Society, 2013, 135, 10950-10953.	6.6	236

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109	Pillar substitution modulates CO2 affinity in â€œmmoâ€•topology networks. Chemical Communications, 2013, 49, 9809.	2.2	47
110	Enhancement of CO2 selectivity in a pillared pcu MOM platform through pillar substitution. Chemical Communications, 2013, 49, 1606.	2.2	87
111	Porous materials with optimal adsorption thermodynamics and kinetics for CO2 separation. Nature, 2013, 495, 80-84.	13.7	2,005
112	Understanding Hydrogen Sorption in a Metalâ€“Organic Framework with Open-Metal Sites and Amide Functional Groups. Journal of Physical Chemistry C, 2013, 117, 9340-9354.	1.5	74
113	Theoretical Investigations of CO₂ and H₂ Sorption in an Interpenetrated Square-Pillared Metalâ€“Organic Material. Journal of Physical Chemistry C, 2013, 117, 9970-9982.	1.5	36
114	Computational Studies of CO₂ Sorption and Separation in an Ultramicroporous Metalâ€“Organic Material. Journal of Physical Chemistry C, 2013, 117, 17687-17698.	1.5	45
115	Examining the Effects of Different Ring Configurations and Equatorial Fluorine Atom Positions on CO₂ Sorption in [Cu(bpy)₂SiF₆]. Crystal Growth and Design, 2013, 13, 4542-4548.	1.4	17
116	A Polarizable and Transferable PHAST CO₂ Potential for Materials Simulation. Journal of Chemical Theory and Computation, 2013, 9, 5421-5429.	2.3	39
117	A Polarizable and Transferable PHAST N₂ Potential for Use in Materials Simulation. Journal of Chemical Theory and Computation, 2013, 9, 5550-5557.	2.3	16
118	Efficient calculation of many-body induced electrostatics in molecular systems. Journal of Chemical Physics, 2013, 139, 184112.	1.2	32
119	Solving the Many-Body Polarization Problem on GPUs: Application to MOFs. Journal of Computational Science Education, 2013, 4, 30-34.	0.3	2
120	A molecular H2 potential for heterogeneous simulations including polarization and many-body van der Waals interactions. Journal of Chemical Physics, 2012, 136, 194302.	1.2	21
121	A theoretical study of the sum frequency vibrational spectroscopy of the carbon tetrachloride/water interface. Journal of Physics Condensed Matter, 2012, 24, 124108.	0.7	3
122	Hydrogen adsorbed in a metal organic framework-5: Coupled translation-rotation eigenstates from quantum five-dimensional calculations. Journal of Chemical Physics, 2012, 137, 014701.	1.2	43
123	Simulation of the Mechanism of Gas Sorption in a Metalâ€“Organic Framework with Open Metal Sites: Molecular Hydrogen in PCN-61. Journal of Physical Chemistry C, 2012, 116, 15538-15549.	1.5	76
124	Highly Selective CO₂ Uptake in Uninodal 6-Connected â€œmmoâ€•Nets Based upon MO₄^{2â€“} (M = Cr, Mo) Pillars. Journal of the American Chemical Society, 2012, 134, 19556-19559.	6.6	110
125	Understanding hydrogen sorption in a polar metal-organic framework with constricted channels. Journal of Chemical Physics, 2012, 136, 034705.	1.2	23
126	Characterization of Tunable Radical Metalâ€“Carbenes: Key Intermediates in Catalytic Cyclopropanation. Organometallics, 2011, 30, 2739-2746.	1.1	73

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127	Dielectric analysis of poly(methyl methacrylate) zinc(II) mono-pinacolborane diphenylporphyrin composites. Polymer, 2010, 51, 4790-4805.	1.8	27
128	Evidence for Substrate Preorganization in the Peptidylglycine Î±-Amidating Monooxygenase Reaction Describing the Contribution of Ground State Structure to Hydrogen Tunneling. Journal of the American Chemical Society, 2010, 132, 16393-16402.	6.6	15
129	Atomic Charges Derived from Electrostatic Potentials for Molecular and Periodic Systems. Journal of Physical Chemistry A, 2010, 114, 10225-10233.	1.1	70
130	A Predictive Model of Hydrogen Sorption for Metalâ^'Organic Materials. Journal of Physical Chemistry C, 2009, 113, 9316-9320.	1.5	41
131	Making a life in the physical sciences. Journal of Organizational Behavior, 2008, 29, 755-759.	2.9	1
132	An Accurate and Transferable Intermolecular Diatomic Hydrogen Potential for Condensed Phase Simulation. Journal of Chemical Theory and Computation, 2008, 4, 1332-1337.	2.3	91
133	Photophysical Studies of the Trans to Cis Isomerization of the Pushâ^'Pull Molecule: 1-(Pyridin-4-yl)-2-(<i>N</i>-methylpyrrol-2-yl)ethene (mepepy). Journal of Physical Chemistry A, 2008, 112, 8310-8315.	1.1	9
134	On the Mechanism of Hydrogen Storage in a Metalâ^'Organic Framework Material. Journal of the American Chemical Society, 2007, 129, 15202-15210.	6.6	182
135	Generalized Computational Time Correlation Function Approach:â€‰ Quantifying Quadrupole Contributions to Vibrationally Resonant Second-Order Interface-Specific Optical Spectroscopiesâ€. Journal of Physical Chemistry C, 2007, 111, 8749-8756.	1.5	11
136	Theoretical Investigation of the Temperature Dependence of the Fifth-Order Raman Response Function of Fluid and Liquid Xenonâ€. Journal of Physical Chemistry B, 2006, 110, 3773-3781.	1.2	13
137	Theoretical Modeling of Interface Specific Vibrational Spectroscopy:â€‰ Methods and Applications to Aqueous Interfaces. Chemical Reviews, 2006, 106, 1234-1258.	23.0	159
138	Time correlation function and finite field approaches to the calculation of the fifth order Raman response in liquid xenon. Journal of Chemical Physics, 2006, 125, 234501.	1.2	18
139	A combined photothermal and molecular dynamics method for determining molecular volume changes. Chemical Physics Letters, 2006, 418, 137-141.	1.2	8
140	A time correlation function theory describing static field enhanced third order optical effects at interfaces. Journal of Chemical Physics, 2006, 125, 224706.	1.2	6
141	Time Correlation Theories of Nonlinear Spectroscopy. , 2006, , 1231-1233.		0
142	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
143	Identification of a wagging vibrational mode of water molecules at the water/vapor interface. Physical Review E, 2005, 71, 050601.	0.8	37
144	Applications of a time correlation function theory for the fifth-order Raman response function I: Atomic liquids. Journal of Chemical Physics, 2005, 123, 194507.	1.2	11

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145	Tractable theory of nonlinear response and multidimensional nonlinear spectroscopy. Physical Review E, 2004, 70, 050101.	0.8	12
146	A time correlation function theory of two-dimensional infrared spectroscopy with applications to liquid water. Journal of Chemical Physics, 2004, 121, 3688-3701.	1.2	38
147	A Molecular Dynamics Study of Aggregation Phenomena in Aqueousn-Propanol. Journal of Physical Chemistry B, 2004, 108, 7389-7401.	1.2	81
148	A Molecular Dynamics Method for Calculating Molecular Volume Changes Appropriate for Biomolecular Simulation. Biophysical Journal, 2003, 85, 2801-2807.	0.2	14
149	A time correlation function theory for the fifth order Raman response function with applications to liquid CS2. Journal of Chemical Physics, 2003, 119, 6073-6082.	1.2	30
150	A combined time correlation function and instantaneous normal mode study of the sum frequency generation spectroscopy of the water/vapor interface. Journal of Chemical Physics, 2003, 118, 8411-8419.	1.2	98
151	A Combined Time Correlation Function and Instantaneous Normal Mode Investigation of Liquid-State Vibrational Spectroscopy. ACS Symposium Series, 2002, , 30-43.	0.5	0
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