Brian Space

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7298688/publications.pdf

Version: 2024-02-01

168	10,975	38742	33894
papers	citations	50 h-index	99 g-index

175	175	175	7205
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Porous materials with optimal adsorption thermodynamics and kinetics for CO2 separation. Nature, 2013, 495, 80-84.	27.8	2,005
2	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.	13.7	383
3	Robust Ultramicroporous Metalâ€“Organic Frameworks with Benchmark Affinity for Acetylene. Angewandte Chemie - International Edition, 2018, 57, 10971-10975.	13.8	365
4	Synergistic sorbent separation for one-step ethylene purification from a four-component mixture. Science, 2019, 366, 241-246.	12.6	360
5	Benchmark C2H2/CO2 and CO2/C2H2 Separation by Two Closely Related Hybrid Ultramicroporous Materials. CheM, 2016, 1, 753-765.	11.7	349
6	A Stable Metalâ€“Organic Framework Featuring a Local Buffer Environment for Carbon Dioxide Fixation. Angewandte Chemie - International Edition, 2018, 57, 4657-4662.	13.8	283
7	Tuning Pore Size in Squareâ€Lattice Coordination Networks for Sizeâ€Selective Sieving of CO₂. Angewandte Chemie - International Edition, 2016, 55, 10268-10272.	13.8	237
8	A Robust Molecular Porous Material with High CO₂ Uptake and Selectivity. Journal of the American Chemical Society, 2013, 135, 10950-10953.	13.7	236
9	On the Mechanism of Hydrogen Storage in a Metalâ^'Organic Framework Material. Journal of the American Chemical Society, 2007, 129, 15202-15210.	13.7	182
10	A Metalâ€“Organic Framework Based Methane Nanoâ€trap for the Capture of Coalâ€Mine Methane. Angewandte Chemie - International Edition, 2019, 58, 10138-10141.	13.8	181
11	A MOFâ€based Ultraâ€Strong Acetylene Nanoâ€trap for Highly Efficient C₂H₂/CO₂ Separation. Angewandte Chemie - International Edition, 2021, 60, 5283-5288.	13.8	172
12	Metalâ€“Organic Framework Based Hydrogen-Bonding Nanotrap for Efficient Acetylene Storage and Separation. Journal of the American Chemical Society, 2022, 144, 1681-1689.	13.7	172
13	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.	13.8	161
14	Theoretical Modeling of Interface Specific Vibrational Spectroscopy:â€‰ Methods and Applications to Aqueous Interfaces. Chemical Reviews, 2006, 106, 1234-1258.	47.7	159
15	Enhanced Gas Uptake in a Microporous Metalâ€“Organic Framework via a Sorbate Induced-Fit Mechanism. Journal of the American Chemical Society, 2019, 141, 17703-17712.	13.7	152
16	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.	4.1	151
17	Trace CO ₂ capture by an ultramicroporous physisorbent with low water affinity. Science Advances, 2019, 5, eaax9171.	10.3	143
18	Hybrid Ultraâ€Microporous Materials for Selective Xenon Adsorption and Separation. Angewandte Chemie - International Edition, 2016, 55, 8285-8289.	13.8	137

#	Article	IF	Citations
19	Effect of ring rotation upon gas adsorption in SIFSIX-3-M (M = Fe, Ni) pillared square grid networks. Chemical Science, 2017, 8, 2373-2380.	7.4	121
20	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.	13.8	119
21	Nonadiabatic dynamics of excited excess electrons in simple fluids. Journal of Chemical Physics, 1991, 94, 1976-1984.	3.0	117
22	Highly Selective Separation of C₂H₂ from CO₂ by a New Dichromate-Based Hybrid Ultramicroporous Material. ACS Applied Materials & Interfaces, 2017, 9, 33395-33400.	8.0	116
23	Hydrophobic pillared square grids for selective removal of CO₂ from simulated flue gas. Chemical Communications, 2015, 51, 15530-15533.	4.1	115
24	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.	13.7	110
25	Putting the Squeeze on CH₄ and CO₂ through Control over Interpenetration in Diamondoid Nets. Journal of the American Chemical Society, 2014, 136, 5072-5077.	13.7	106
26	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.	3.0	98
27	An Accurate and Transferable Intermolecular Diatomic Hydrogen Potential for Condensed Phase Simulation. Journal of Chemical Theory and Computation, 2008, 4, 1332-1337.	5.3	91
28	Dynamics of trapping and localization of excess electrons in simple fluids. Journal of Chemical Physics, 1992, 96, 652-663.	3.0	87
29	Enhancement of CO2 selectivity in a pillared pcu MOM platform through pillar substitution. Chemical Communications, 2013, 49, 1606.	4.1	87
30	Robust Ultramicroporous Metalâ€“Organic Frameworks with Benchmark Affinity for Acetylene. Angewandte Chemie, 2018, 130, 11137-11141.	2.0	85
31	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.	3.1	84
32	A Molecular Dynamics Study of Aggregation Phenomena in Aqueousn-Propanol. Journal of Physical Chemistry B, 2004, 108, 7389-7401.	2.6	81
33	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.	3.1	76
34	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.	3.1	74
35	Characterization of Tunable Radical Metalâ€“Carbenes: Key Intermediates in Catalytic Cyclopropanation. Organometallics, 2011, 30, 2739-2746.	2.3	73
36	Remote Stabilization of Copper Paddlewheel Based Molecular Building Blocks in Metalâ€“Organic Frameworks. Chemistry of Materials, 2015, 27, 2144-2151.	6.7	72

#	Article	IF	Citations
37	Halogenâ€“C₂H₂ Binding in Ultramicroporous Metalâ€“Organic Frameworks (MOFs) for Benchmark C₂H₂/CO₂ Separation Selectivity. Chemistry - A European Journal, 2020, 26, 4923-4929.	3.3	72
38	Atomic Charges Derived from Electrostatic Potentials for Molecular and Periodic Systems. Journal of Physical Chemistry A, 2010, 114, 10225-10233.	2.5	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.	13.8	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.	3.0	68
41	Breaking the trade-off between selectivity and adsorption capacity for gas separation. CheM, 2021, 7, 3085-3098.	11.7	68
42	Crystal engineering of a family of hybrid ultramicroporous materials based upon interpenetration and dichromate linkers. Chemical Science, 2016, 7, 5470-5476.	7.4	66
43	One-step ethylene production from a four-component gas mixture by a single physisorbent. Nature Communications, 2021, 12, 6507.	12.8	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.	3.0	63
45	Readily accessible shape-memory effect in a porous interpenetrated coordination network. Science Advances, 2018, 4, eaaq1636.	10.3	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.	13.8	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.	13.8	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.	3.0	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.	10.3	55
50	Radiation-resistant metal-organic framework enables efficient separation of krypton fission gas from spent nuclear fuel. Nature Communications, 2020, 11, 3103.	12.8	54
51	Efficient CO₂ Removal for Ultraâ€Pure CO Production by Two Hybrid Ultramicroporous Materials. Angewandte Chemie - International Edition, 2018, 57, 3332-3336.	13.8	52
52	Towards an understanding of the propensity for crystalline hydrate formation by molecular compounds. IUCrJ, 2016, 3, 430-439.	2.2	49
53	A MOFâ€based Ultraâ€Strong Acetylene Nanoâ€trap for Highly Efficient C₂H₂/CO₂ Separation. Angewandte Chemie, 2021, 133, 5343-5348.	2.0	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.	4.1	48

#	Article	IF	Citations
55	Pillar substitution modulates CO2 affinity in â€œmmoâ€•topology networks. Chemical Communications, 2013, 49, 9809.	4.1	47
56	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.	4.1	47
57	Selfâ€Adjusting Metalâ€“Organic Framework for Efficient Capture of Trace Xenon and Krypton. Angewandte Chemie - International Edition, 2022, 61, .	13.8	47
58	Computational Studies of CO₂ Sorption and Separation in an Ultramicroporous Metalâ€“Organic Material. Journal of Physical Chemistry C, 2013, 117, 17687-17698.	3.1	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 Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2021, 143, 12202-12211.	13.7	44
60	Hydrogen adsorbed in a metal organic framework-5: Coupled translation-rotation eigenstates from quantum five-dimensional calculations. Journal of Chemical Physics, 2012, 137, 014701.	3.0	43
61	Tuning Pore Size in Squareâ€Lattice Coordination Networks for Sizeâ€Selective Sieving of CO₂. Angewandte Chemie, 2016, 128, 10424-10428.	2.0	43
62	Vibrationally resolved shape resonant photoionization of N2O. Journal of Chemical Physics, 1989, 90, 1544-1550.	3.0	42
63	Long time scale molecular dynamics subspace integration method applied to anharmonic crystals and glasses. Journal of Chemical Physics, 1993, 99, 9070-9079.	3.0	42
64	A Predictive Model of Hydrogen Sorption for Metalâˆ’Organic Materials. Journal of Physical Chemistry C, 2009, 113, 9316-9320.	3.1	41
65	Investigating the Gas Sorption Mechanism in an rht-Metalâ€“Organic Framework through Computational Studies. Journal of Physical Chemistry C, 2014, 118, 439-456.	3.1	40
66	Capturing the H₂â€“Metal Interaction in Mg-MOF-74 Using Classical Polarization. Journal of Physical Chemistry C, 2014, 118, 22683-22690.	3.1	40
67	The effect of centred versus offset interpenetration on C₂H₂ sorption in hybrid ultramicroporous materials. Chemical Communications, 2017, 53, 11592-11595.	4.1	40
68	A robust soc-MOF platform exhibiting high gravimetric uptake and volumetric deliverable capacity for on-board methane storage. Nano Research, 2021, 14, 512-517.	10.4	40
69	A Polarizable and Transferable PHAST CO₂ Potential for Materials Simulation. Journal of Chemical Theory and Computation, 2013, 9, 5421-5429.	5.3	39
70	A combined instantaneous normal mode and time correlation function description of the optical Kerr effect and Raman spectroscopy of liquid CS2. Journal of Chemical Physics, 2000, 112, 4186-4192.	3.0	38
71	A time correlation function theory of two-dimensional infrared spectroscopy with applications to liquid water. Journal of Chemical Physics, 2004, 121, 3688-3701.	3.0	38
72	Hybrid Ultraâ€Microporous Materials for Selective Xenon Adsorption and Separation. Angewandte Chemie, 2016, 128, 8425-8429.	2.0	38

#	Article	IF	Citations
73	Impact of partial interpenetration in a hybrid ultramicroporous material on C₂H₂/C₂H₄ separation performance. Chemical Communications, 2018, 54, 3488-3491.	4.1	38
74	Identification of a wagging vibrational mode of water molecules at the water/vapor interface. Physical Review E, 2005, 71, 050601.	2.1	37
75	Theoretical Investigations of CO₂ and H₂ Sorption in an Interpenetrated Square-Pillared Metalâ€“Organic Material. Journal of Physical Chemistry C, 2013, 117, 9970-9982.	3.1	36
76	Theoretical Investigations of CO₂ and CH₄ Sorption in an Interpenetrated Diamondoid Metalâ€“Organic Material. Langmuir, 2014, 30, 6454-6462.	3.5	35
77	Investigating CO₂ Sorption in SIFSIX-3-M (M = Fe, Co, Ni, Cu, Zn) through Computational Studies. Crystal Growth and Design, 2019, 19, 3732-3743.	3.0	35
78	Fine Tuning of MOFâ€505 Analogues To Reduce Lowâ€Pressure Methane Uptake and Enhance Methane Working Capacity. Angewandte Chemie, 2017, 129, 11584-11588.	2.0	33
79	Efficient calculation of many-body induced electrostatics in molecular systems. Journal of Chemical Physics, 2013, 139, 184112.	3.0	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.	3.0	32
81	A Stable Metalâ€“Organic Framework Featuring a Local Buffer Environment for Carbon Dioxide Fixation. Angewandte Chemie, 2018, 130, 4747-4752.	2.0	32
82	Highly selective CO₂ removal for one-step liquefied natural gas processing by physisorbents. Chemical Communications, 2019, 55, 3219-3222.	4.1	31
83	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.	3.0	30
84	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.	8.0	30
85	An instantaneous normal mode theory of condensed phase absorption: The collision-induced absorption spectra of liquid CO2. Journal of Chemical Physics, 1997, 107, 5635-5644.	3.0	29
86	Metal-organic materials with triazine-based ligands: From structures to properties and applications. Coordination Chemistry Reviews, 2021, 427, 213518.	18.8	29
87	A high rotational barrier for physisorbed hydrogen in an fcu-metalâ€“organic framework. Chemical Communications, 2014, 50, 14109-14112.	4.1	28
88	A Metalâ€“Organic Framework Based Methane Nanoâ€trap for the Capture of Coalâ€Mine Methane. Angewandte Chemie, 2019, 131, 10244-10247.	2.0	28
89	Indiumâ€“Organic Framework with soc Topology as a Versatile Catalyst for Highly Efficient One-Pot Strecker Synthesis of Î±-aminonitriles. ACS Applied Materials & Interfaces, 2021, 13, 52023-52033.	8.0	28
90	Ultramicropore Engineering by Dehydration to Enable Molecular Sieving of H₂ by Calcium Trimesate. Angewandte Chemie - International Edition, 2020, 59, 16188-16194.	13.8	28

#	Article	IF	Citations
91	Dielectric analysis of poly(methyl methacrylate) zinc(II) mono-pinacolborane diphenylporphyrin composites. Polymer, 2010, 51, 4790-4805.	3.8	27
92	Dramatic effect of pore size reduction on the dynamics of hydrogen adsorbed in metalâ€“organic materials. Journal of Materials Chemistry A, 2014, 2, 13884.	10.3	27
93	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.	2.0	27
94	Investigating H2Sorption in a Fluorinated Metalâ€“Organic Framework with Small Pores Through Molecular Simulation and Inelastic Neutron Scattering. Langmuir, 2015, 31, 7328-7336.	3.5	26
95	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.	8.0	26
96	Efficient propyne/propadiene separation by microporous crystalline physiadsorbents. Nature Communications, 2021, 12, 5768.	12.8	26
97	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.	2.8	24
98	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.	2.8	24
99	A theoretical investigation of the temperature dependence of the optical Kerr effect and Raman spectroscopy of liquid CS2. Journal of Chemical Physics, 2000, 113, 8693-8699.	3.0	23
100	Understanding hydrogen sorption in a polar metal-organic framework with constricted channels. Journal of Chemical Physics, 2012, 136, 034705.	3.0	23
101	Modeling PCN-61 and PCN-66: Isostructural rht-Metalâ€“Organic Frameworks with Distinct CO₂ Sorption Mechanisms. Crystal Growth and Design, 2014, 14, 5599-5607.	3.0	23
102	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.	2.8	23
103	Dramatic Effect of the Electrostatic Parameters on H2 Sorption in an M-MOF-74 Analogue. Crystal Growth and Design, 2016, 16, 867-874.	3.0	23
104	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.	4.0	23
105	Feasibility of using photophoresis to create a concentration gradient of solvated molecules. Journal of Chemical Physics, 1996, 105, 9515-9524.	3.0	22
106	Comparing the mechanism and energetics of CO₂ sorption in the SIFSIX series. CrystEngComm, 2017, 19, 3338-3347.	2.6	22
107	A robust heterometallic ultramicroporous MOF with ultrahigh selectivity for propyne/propylene separation. Journal of Materials Chemistry A, 2021, 9, 2850-2856.	10.3	22
108	Vibrationally resolved electronic autoionization of coreâ€“hole resonances. Journal of Chemical Physics, 1988, 89, 4048-4053.	3.0	21

#	Article	IF	Citations
109	Subspace Method for Long Time Scale Molecular Dynamics. The Journal of Physical Chemistry, 1995, 99, 7330-7338.	2.9	21
110	A molecular H2 potential for heterogeneous simulations including polarization and many-body van der Waals interactions. Journal of Chemical Physics, 2012, 136, 194302.	3.0	21
111	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.	3.0	21
112	Experimental and theoretical investigations of the gas adsorption sites in rht-metalâ€“organic frameworks. CrystEngComm, 2017, 19, 4646-4665.	2.6	20
113	An instantaneous normal mode theory of condensed phase absorption: the vibrational spectrum of condensed CS2 from boiling to freezing. Chemical Physics Letters, 1998, 296, 259-265.	2.6	18
114	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.	3.0	18
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.	3.0	17
116	Accurate H₂ Sorption Modeling in the rht-MOF NOTT-112 Using Explicit Polarization. Crystal Growth and Design, 2016, 16, 6024-6032.	3.0	17
117	Theoretical Investigations of CO₂ and H₂ Sorption in Robust Molecular Porous Materials. Langmuir, 2016, 32, 11492-11505.	3.5	17
118	The rotational dynamics of H₂ adsorbed in covalent organic frameworks. Physical Chemistry Chemical Physics, 2017, 19, 13075-13082.	2.8	17
119	Hydrogen Adsorption in a Zeolitic Imidazolate Framework with lta Topology. Journal of Physical Chemistry C, 2018, 122, 15435-15445.	3.1	17
120	A Polarizable and Transferable PHAST N₂ Potential for Use in Materials Simulation. Journal of Chemical Theory and Computation, 2013, 9, 5550-5557.	5.3	16
121	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.	4.1	16
122	Robust Microporous Metalâ€“Organic Frameworks for Highly Efficient and Simultaneous Removal of Propyne and Propadiene from Propylene. Angewandte Chemie, 2019, 131, 10315-10320.	2.0	16
123	Insights into the Gas Adsorption Mechanisms in Metalâ€“Organic Frameworks from Classical Molecular Simulations. Topics in Current Chemistry, 2020, 378, 14.	5.8	16
124	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.	13.7	15
125	Simulations of hydrogen, carbon dioxide, and small hydrocarbon sorption in a nitrogen-rich rht-metalâ€“organic framework. Physical Chemistry Chemical Physics, 2018, 20, 1761-1777.	2.8	15
126	A Molecular Dynamics Method for Calculating Molecular Volume Changes Appropriate for Biomolecular Simulation. Biophysical Journal, 2003, 85, 2801-2807.	0.5	14

#	Article	IF	Citations
127	Theoretical Insights into the Tuning of Metal Binding Sites of Paddlewheels in rhtâ€Metalâ€“Organic Frameworks. ChemPhysChem, 2015, 16, 3170-3179.	2.1	14
128	Benchmark Acetylene Binding Affinity and Separation through Induced Fit in a Flexible Hybrid Ultramicroporous Material. Angewandte Chemie, 2021, 133, 20546-20553.	2.0	14
129	Interchannel interactions following shape resonant excitation of core electrons. Chemical Physics, 1989, 129, 65-71.	1.9	13
130	A Novel Technique for the Measurement of Polarization-Specific Ultrafast Raman Responses. Journal of Physical Chemistry A, 2001, 105, 9851-9858.	2.5	13
131	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.	2.6	13
132	High H₂ Sorption Energetics in Zeolitic Imidazolate Frameworks. Journal of Physical Chemistry C, 2017, 121, 1723-1733.	3.1	13
133	Toward an Understanding of the Propensity for Crystalline Hydrate Formation by Molecular Compounds. Part 2. Crystal Growth and Design, 2021, 21, 4927-4939.	3.0	13
134	Tractable theory of nonlinear response and multidimensional nonlinear spectroscopy. Physical Review E, 2004, 70, 050101.	2.1	12
135	Efficient CO₂ Removal for Ultraâ€Pure CO Production by Two Hybrid Ultramicroporous Materials. Angewandte Chemie, 2018, 130, 3390-3394.	2.0	12
136	Applications of a time correlation function theory for the fifth-order Raman response function I: Atomic liquids. Journal of Chemical Physics, 2005, 123, 194507.	3.0	11
137	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.	3.1	11
138	An unusual H2 sorption mechanism in PCN-14: insights from molecular simulation. Physical Chemistry Chemical Physics, 2016, 18, 21421-21430.	2.8	11
139	Inelastic Neutron Scattering and Theoretical Studies of H2Sorption in a Dy(III)-Based Phosphine Coordination Material. Chemistry of Materials, 2015, 27, 7619-7626.	6.7	10
140	Aminoâ€Functionalised Hybrid Ultramicroporous Materials that Enable Singleâ€Step Ethylene Purification from a Ternary Mixture. Angewandte Chemie, 2021, 133, 10997-11004.	2.0	10
141	An atomically detailed description of metalâ€“dielectric interfaces: The crossover from surface to bulk conducting properties of Agâ€“Xe. Journal of Chemical Physics, 2000, 112, 10998-11004.	3.0	9
142	Photophysical Studies of the Trans to Cis Isomerization of the Pushâ^'Pull Molecule: 1-(Pyridin-4-yl)-2-(N-methylpyrrol-2-yl)ethene (mepepy). Journal of Physical Chemistry A, 2008, 112, 8310-8315.	2.5	9
143	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.	3.0	9
144	Tuning the Selectivity between C2H2 and CO2 in Molecular Porous Materials. Langmuir, 2021, 37, 13838-13845.	3.5	9

#	Article	IF	Citations
145	A combined photothermal and molecular dynamics method for determining molecular volume changes. Chemical Physics Letters, 2006, 418, 137-141.	2.6	8
146	Investigating gas sorption in an rht-metalâ€“organic framework with 1,2,3-triazole groups. Physical Chemistry Chemical Physics, 2017, 19, 29204-29221.	2.8	8
147	MPMC and MCMD: Free Highâ€Performance Simulation Software for Atomistic Systems. Advanced Theory and Simulations, 2019, 2, 1900113.	2.8	8
148	Ultramicropore Engineering by Dehydration to Enable Molecular Sieving of H 2 by Calcium Trimesate. Angewandte Chemie, 2020, 132, 16322-16328.	2.0	8
149	Methane storage in flexible and dynamical metalâ€“organic frameworks. Chemical Physics Reviews, 2022, 3, .	5.7	7
150	A time correlation function theory describing static field enhanced third order optical effects at interfaces. Journal of Chemical Physics, 2006, 125, 224706.	3.0	6
151	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.	2.6	5
152	Next-Generation Accurate, Transferable, and Polarizable Potentials for Material Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7632-7644.	5.3	5
153	Selfâ€Adjusting Metalâ€“Organic Framework for Efficient Capture of Trace Xenon and Krypton. Angewandte Chemie, 2022, 134, .	2.0	5
154	Investigating H₂ Adsorption in Isostructural Metalâ€“Organic Frameworks M-CUK-1 (M = Co) Tj ETQq0 0 0 rgBT /Overlock 14, 8126-8136.	8.0	5
155	The effective mass of excess electrons in condensed xenon: Toward methods for modeling metal-dielectric interfaces. Journal of Chemical Physics, 1997, 107, 1922-1930.	3.0	4
156	A theoretical study of the sum frequency vibrational spectroscopy of the carbon tetrachloride/water interface. Journal of Physics Condensed Matter, 2012, 24, 124108.	1.8	3
157	Investigating C₂H₂ Sorption in Î±-[M₃(O₂CH)₆] (M = Mg, Mn) Through Theoretical Studies. Crystal Growth and Design, 2018, 18, 5342-5352.	3.0	2
158	Insights into the Gas Adsorption Mechanisms in Metalâ€“Organic Frameworks from Classical Molecular Simulations. Topics in Current Chemistry Collections, 2020, , 215-279.	0.5	2
159	Solving the Many-Body Polarization Problem on GPUs: Application to MOFs. Journal of Computational Science Education, 2013, 4, 30-34.	0.3	2
160	Making a life in the physical sciences. Journal of Organizational Behavior, 2008, 29, 755-759.	4.7	1
161	Simulations of H₂ Sorption in an Anthracene-Functionalized rht-Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2020, 124, 13753-13764.	3.1	1
162	Frontispiz: A MOFâ€based Ultraâ€Strong Acetylene Nanoâ€trap for Highly Efficient C₂H₂/CO₂ Separation. Angewandte Chemie, 2021, 133, .	2.0	1

#	Article	IF	Citations
163	Theoretical study of the effect of halogen substitution in molecular porous materials for CO₂ and C₂H₂ sorption. AIMS Materials Science, 2018, 5, 226-245.	1.4	1
164	A Combined Time Correlation Function and Instantaneous Normal Mode Investigation of Liquid-State Vibrational Spectroscopy. ACS Symposium Series, 2002, , 30-43.	0.5	0
165	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.	2.0	0
166	Innentitelbild: Ultramicropore Engineering by Dehydration to Enable Molecular Sieving of H₂ by Calcium Trimesate (Angew. Chem. 37/2020). Angewandte Chemie, 2020, 132, 15898-15898.	2.0	0
167	Frontispiece: A MOFâ€based Ultraâ€Strong Acetylene Nanoâ€trap for Highly Efficient C₂H₂/CO₂ Separation. Angewandte Chemie - International Edition, 2021, 60, .	13.8	0
168	Time Correlation Theories of Nonlinear Spectroscopy. , 2006, , 1231-1233.		0