Sofia Calero

List of Publications by Year
in descending order

216 papers	9,747 citations	30047 54 h-index	49868 87 g-index
230 all docs	230 docs citations	230 times ranked	7314 citing authors

#	Article	IF	Citations
1	Water adsorption in ideal and defective UiO-66 structures. Microporous and Mesoporous Materials, 2022, 330, 111555.	2.2	28
2	Transitioning from Ionic Liquids to Deep Eutectic Solvents. ACS Sustainable Chemistry and Engineering, 2022, 10, 1232-1245.	3.2	22
3	Thermostructural Characterization of Silicon Carbide Nanocomposite Materials via Molecular Dynamics Simulations. Advanced Composite Materials, 2022, 31, 485-504.	1.0	0
4	Challenges of modeling nanostructured materials for photocatalytic water splitting. Chemical Society Reviews, 2022, 51, 3794-3818.	18.7	64
5	Adsorption of Linear Alcohols in Amorphous Activated Carbons: Implications for Energy Storage Applications. ACS Sustainable Chemistry and Engineering, 2022, 10, 6509-6520.	3.2	5
6	Revisiting Vibrational Spectroscopy to Tackle the Chemistry of Zr₆O₈ Metal-Organic Framework Nodes. ACS Applied Materials & Interfaces, 2022, 14, 27040-27047.	4.0	7
7	Separation of Volatile Organic Compounds in TAMOF-1. ACS Applied Materials & Interfaces, 2022, 14, 30772-30785.	4.0	3
8	Enhancing separation efficiency in European syngas industry by using zeolites. Catalysis Today, 2021, 362, 113-121.	2.2	10
9	High-throughput screening of metal â€“ Organic frameworks for CO2 and CH4 separation in the presence of water. Chemical Engineering Journal, 2021, 403, 126392.	6.6	53
10	Potential of CO2 capture from flue gases by physicochemical and biological methods: A comparative study. Chemical Engineering Journal, 2021, 417, 128020.	6.6	17
11	Effect of diol isomer/water mixtures on the stability of Zn-MOF-74. Dalton Transactions, 2021, 50, 1808-1815.	1.6	3
12	In Silico Screening of Zeolites for High-Pressure Hydrogen Drying. ACS Applied Materials & Interfaces, 2021, 13, 8383-8394.	4.0	7
13	New Features of the Open Source Monte Carlo Software Brick-CFCMC: Thermodynamic Integration and Hybrid Trial Moves. Journal of Chemical Information and Modeling, 2021, 61, 3752-3757.	2.5	14
14	Carbon Dioxide Capture Enhanced by Preâ€Adsorption of Water and Methanol in UiOâ€66. Chemistry - A European Journal, 2021, 27, 14653-14659.	1.7	17
15	On the design of models for an accurate description of the water â€“ hematite interface. Applied Surface Science, 2021, 560, 149884.	3.1	1
16	EMIMBF4 in ternary liquid mixtures of water, dimethyl sulfoxide and acetonitrile as â€œtri-solvent-in-saltâ€•electrolytes for high-performance supercapacitors operating at -70ÂÂ°C. Energy Storage Materials, 2021, 40, 368-385.	9.5	25
17	The role of hydrogen bonding in the dehydration of bioalcohols in hydrophobic pervaporation membranes. Journal of Molecular Liquids, 2021, 340, 117297.	2.3	5
18	Modifying the hydrophobic nature of MAF-6. Separation and Purification Technology, 2021, 277, 119422.	3.9	3

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19	Metastable Zr/Hf-MOFs: the hexagonal family of EHU-30 and their water-sorption induced structural transformation. Inorganic Chemistry Frontiers, 2021, 8, 4767-4779.	3.0	8
20	Ï€-Complexation for olefin/paraffin separation using aluminosilicates. Chemical Engineering Journal, 2020, 380, 122482.	6.6	28
21	Role of hydrogen bonding in the capture and storage of ammonia in zeolites. Chemical Engineering Journal, 2020, 387, 124062.	6.6	37
22	Effect of lattice shrinking on the migration of water within zeolite LTA. Microporous and Mesoporous Materials, 2020, 293, 109808.	2.2	9
23	Computational Approaches to Zeolite-Based Adsorption Processes. Structure and Bonding, 2020, , 57-83.	1.0	2
24	Impact of Small Adsorbates in the Vibrational Spectra of Mg- and Zn-MOF-74 Revealed by First-Principles Calculations. ACS Applied Materials & Interfaces, 2020, 12, 54980-54990.	4.0	14
25	Aqueous Coâ€Solvent in Zwitterionicâ€based Protic Ionic Liquids as Electrolytes in 2.0â€…V Supercapacitors. ChemSusChem, 2020, 13, 5983-5995.	3.6	8
26	Exploiting the Ï€-bonding for the separation of benzene and cyclohexane in zeolites. Chemical Engineering Journal, 2020, 398, 125678.	6.6	23
27	Efficient modelling of ion structure and dynamics in inorganic metal halide perovskites. Journal of Materials Chemistry A, 2020, 8, 11824-11836.	5.2	26
28	OCEAN: An Algorithm to Predict the Separation of Biogas Using Zeolites. Industrial & Engineering Chemistry Research, 2020, 59, 7212-7223.	1.8	7
29	Further Extending the Dilution Range of the â€œSolvent-in-DESâ€•Regime upon the Replacement of Water by an Organic Solvent with Hydrogen Bond Capabilities. ACS Sustainable Chemistry and Engineering, 2020, 8, 12120-12131.	3.2	20
30	Homochiral Metalâ€“Organic Frameworks for Enantioselective Separations in Liquid Chromatography. Journal of the American Chemical Society, 2019, 141, 14306-14316.	6.6	93
31	Using Aliphatic Alcohols to Tune Benzene Adsorption in MAFâ€6. Advanced Theory and Simulations, 2019, 2, 1900112.	1.3	1
32	Acetylene Storage and Separation Using Metalâ€“Organic Frameworks with Open Metal Sites. ACS Applied Materials & Interfaces, 2019, 11, 31499-31507.	4.0	43
33	Improving Ammonia Production Using Zeolites. Journal of Physical Chemistry C, 2019, 123, 18475-18481.	1.5	16
34	Looking at the â€œWater-in-Deep-Eutectic-Solventâ€•System: A Dilution Range for High Performance Eutectics. ACS Sustainable Chemistry and Engineering, 2019, 7, 17565-17573.	3.2	80
35	Design, Parameterization, and Implementation of Atomic Force Fields for Adsorption in Nanoporous Materials. Advanced Theory and Simulations, 2019, 2, 1900135.	1.3	41
36	Adsorption of Light Alcohols in a High Hydrophobic Metal Azolate Framework. Journal of Physical Chemistry C, 2019, 123, 23987-23994.	1.5	5

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37	Intermediate states approach for adsorption studies in flexible metalâ€“organic frameworks. Physical Chemistry Chemical Physics, 2019, 21, 3294-3303.	1.3	13
38	Enhancing the Water Capacity in Zr-Based Metalâ€“Organic Framework for Heat Pump and Atmospheric Water Generator Applications. ACS Applied Nano Materials, 2019, 2, 3050-3059.	2.4	18
39	Molecular Sieves for the Separation of Hydrogen Isotopes. ACS Applied Materials & Interfaces, 2019, 11, 18833-18840.	4.0	36
40	Highlights of (bio-)chemical tools and visualization software for computational science. Current Opinion in Chemical Engineering, 2019, 23, 1-13.	3.8	7
41	Adsorption of Alkanes in Zeolites LTA and FAU: Quasi-Equilibrated Thermodesorption Supported by Molecular Simulations. Journal of Physical Chemistry C, 2019, 123, 29665-29678.	1.5	7
42	Adsorption and Diffusion of Benzene in Mg-MOF-74 with Open Metal Sites. ACS Applied Materials & Interfaces, 2019, 11, 4686-4700.	4.0	46
43	Improving Olefin Purification Using Metal Organic Frameworks with Open Metal Sites. ACS Applied Materials & Interfaces, 2018, 10, 16911-16917.	4.0	25
44	Phase Transition Induced by Gas Adsorption in Metalâ€Organic Frameworks. Chemistry - A European Journal, 2018, 24, 8530-8534.	1.7	15
45	Unravelling the influence of carbon dioxide on the adsorptive recovery of butanol from fermentation broth using ITQ-29 and ZIF-8. Physical Chemistry Chemical Physics, 2018, 20, 9957-9964.	1.3	16
46	Stepped Propane Adsorption in Pure-Silica ITW Zeolite. Langmuir, 2018, 34, 4774-4779.	1.6	10
47	iRASPA: GPU-accelerated visualization software for materials scientists. Molecular Simulation, 2018, 44, 653-676.	0.9	112
48	Influence of Flexibility on the Separation of Chiral Isomers in STWâ€Type Zeolite. Chemistry - A European Journal, 2018, 24, 4121-4132.	1.7	14
49	Adsorption equilibrium of nitrogen dioxide in porous materials. Physical Chemistry Chemical Physics, 2018, 20, 4189-4199.	1.3	20
50	Molecular Dynamics Analysis of Charge Transport in Ionicâ€Liquid Electrolytes Containing Added Salt with Mono, Di, and Trivalent Metal Cations. ChemPhysChem, 2018, 19, 1665-1673.	1.0	23
51	Effect of Light Gases in the Ethane/Ethylene Separation Using Zeolitic Imidazolate Frameworks. Journal of Physical Chemistry C, 2018, 122, 8637-8646.	1.5	8
52	Potential of polarizable force fields for predicting the separation performance of small hydrocarbons in M-MOF-74. Physical Chemistry Chemical Physics, 2018, 20, 28848-28859.	1.3	18
53	Diffusion Patterns in Zeolite MFI: The Cation Effect. Journal of Physical Chemistry C, 2018, 122, 29274-29284.	1.5	6
54	Adsorption of Cyclohexane in Pure Silica Zeolites: Highâ€Throughput Computational Screening Validated by Experimental Data. ChemPhysChem, 2018, 19, 3364-3371.	1.0	8

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55	Zeolites for CO₂â€“COâ€“O₂ Separation to Obtain CO₂-Neutral Fuels. ACS Applied Materials & Interfaces, 2018, 10, 20512-20520.	4.0	30
56	Identifying Zeolite Topologies for Storage and Release of Hydrogen. Journal of Physical Chemistry C, 2018, 122, 12485-12493.	1.5	20
57	The Siâ€“Ge substitutional series in the chiral STW zeolite structure type. Journal of Materials Chemistry A, 2018, 6, 15110-15122.	5.2	33
58	Gate-Opening Mechanism of Hydrophilicâ€“Hydrophobic Metalâ€“Organic Frameworks: Molecular Simulations and Quasi-Equilibrated Desorption. Chemistry of Materials, 2018, 30, 5116-5127.	3.2	17
59	Role of Ionic Liquid [EMIM]⁺[SCN]^{â^'} in the Adsorption and Diffusion of Gases in Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2018, 10, 29694-29704.	4.0	38
60	Fitting electron density as a physically sound basis for the development of interatomic potentials of complex alloys. Physical Chemistry Chemical Physics, 2018, 20, 18647-18656.	1.3	2
61	Discovery of an Optimal Porous Crystalline Material for the Capture of Chemical Warfare Agents. Chemistry of Materials, 2018, 30, 4571-4579.	3.2	62
62	Importance of Blocking Inaccessible Voids on Modeling Zeolite Adsorption: Revisited. Journal of Physical Chemistry C, 2017, 121, 4462-4470.	1.5	17
63	Adsorptive process design for the separation of hexane isomers using zeolites. Physical Chemistry Chemical Physics, 2017, 19, 5037-5042.	1.3	24
64	Effective Model for Olefin/Paraffin Separation using (Co, Fe, Mn, Ni)â€MOFâ€74. ChemistrySelect, 2017, 2, 665-672.	0.7	16
65	Selective sulfur dioxide adsorption on crystal defect sites on an isoreticular metal organic framework series. Nature Communications, 2017, 8, 14457.	5.8	133
66	Adsorptive separation of ethane and ethylene using IsoReticular Metal-Organic Frameworks. Microporous and Mesoporous Materials, 2017, 248, 40-45.	2.2	20
67	Porphyrin-based metal-organic frameworks for solar fuel synthesis photocatalysis: band gap tuning via iron substitutions. Journal of Materials Chemistry A, 2017, 5, 11894-11904.	5.2	84
68	Ordering of n-Alkanes Adsorbed in the Micropores of AlPO₄-5: A Combined Molecular Simulations and Quasi-Equilibrated Thermodesorption Study. Journal of Physical Chemistry C, 2017, 121, 25292-25302.	1.5	16
69	Quasi-Equilibrated Thermodesorption Combined with Molecular Simulation for Adsorption and Separation of Hexane Isomers in Zeolites MFI and MEL. Journal of Physical Chemistry C, 2017, 121, 19226-19238.	1.5	11
70	Micelle Formation in Aqueous Solutions of Room Temperature Ionic Liquids: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2017, 121, 8348-8358.	1.2	39
71	Tuning the separation properties of zeolitic imidazolate framework coreâ€“shell structures via post-synthetic modification. Journal of Materials Chemistry A, 2017, 5, 25601-25608.	5.2	56
72	Cadmiumâ€“BINOL Metalâ€“Organic Framework for the Separation of Alcohol Isomers. Chemistry - A European Journal, 2017, 23, 874-885.	1.7	12

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73	On the molecular mechanisms for the H₂/CO₂ separation performance of zeolite imidazolate framework two-layered membranes. Chemical Science, 2017, 8, 325-333.	3.7	91
74	Olefin/Paraffin Separation in Open Metal Site Cu-BTC Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2017, 121, 3126-3132.	1.5	37
75	Critical Role of Dynamic Flexibility in Geâ€Containing Zeolites: Impact on Diffusion. Chemistry - A European Journal, 2016, 22, 10036-10043.	1.7	22
76	Frontispiece: Modelling a Linker Mixâ€andâ€Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. Angewandte Chemie - International Edition, 2016, 55, .	7.2	1
77	Storage and Separation of Carbon Dioxide and Methane in Hydrated Covalent Organic Frameworks. Journal of Physical Chemistry C, 2016, 120, 23756-23762.	1.5	36
78	Impact of the Nature of Exchangeable Cations on LTA-Type Zeolite Hydration. Journal of Physical Chemistry C, 2016, 120, 23254-23261.	1.5	19
79	Modelling a Linker Mixâ€andâ€Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. Angewandte Chemie - International Edition, 2016, 55, 16012-16016.	7.2	61
80	Modelling a Linker Mixâ€andâ€Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. Angewandte Chemie, 2016, 128, 16246-16250.	1.6	12
81	Highly Selective Zeolite Topologies for Flue Gas Separation. Chemistry - A European Journal, 2016, 22, 18705-18708.	1.7	16
82	Controlling Thermal Expansion: A Metalâ€“Organic Frameworks Route. Chemistry of Materials, 2016, 28, 8296-8304.	3.2	42
83	Adsorption of n-Alkanes in MFI and MEL: Quasi-Equilibrated Thermodesorption Combined with Molecular Simulations. Journal of Physical Chemistry C, 2016, 120, 25338-25350.	1.5	18
84	Aqueous Solutions of Ionic Liquids: Microscopic Assembly. ChemPhysChem, 2016, 17, 380-386.	1.0	14
85	Liquid self-diffusion of H₂O and DMF molecules in Co-MOF-74: molecular dynamics simulations and dielectric spectroscopy studies. Physical Chemistry Chemical Physics, 2016, 18, 19605-19612.	1.3	21
86	Quantum and Classical Molecular Dynamics of Ionic Liquid Electrolytes for Na/Liâ€based Batteries: Molecular Origins of the Conductivity Behavior. ChemPhysChem, 2016, 17, 2473-2481.	1.0	29
87	Comparing gas separation performance between all known zeolites and their zeolitic imidazolate framework counterparts. Dalton Transactions, 2016, 45, 216-225.	1.6	26
88	Computing bubble-points of CO2/CH4 gas mixtures in ionic liquids from Monte Carlo simulations. Fluid Phase Equilibria, 2016, 418, 100-107.	1.4	9
89	Solubilities of CO2, CH4, C2H6, and SO2 in ionic liquids and Selexol from Monte Carlo simulations. Journal of Computational Science, 2016, 15, 74-80.	1.5	31
90	RASPA: molecular simulation software for adsorption and diffusion in flexible nanoporous materials. Molecular Simulation, 2016, 42, 81-101.	0.9	1,266

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91	Separation of Amyl Alcohol Isomers in ZIFâ€77. ChemPhysChem, 2015, 16, 2735-2738.	1.0	8
92	Selective Adsorption of Water from Mixtures with 1-Alcohols by Exploitation of Molecular Packing Effects in CuBTC. Journal of Physical Chemistry C, 2015, 119, 3658-3666.	1.5	29
93	Molecular dynamics simulations of organohalide perovskite precursors: solvent effects in the formation of perovskite solar cells. Physical Chemistry Chemical Physics, 2015, 17, 22770-22777.	1.3	32
94	Zeolites for the selective adsorption of sulfur hexafluoride. Physical Chemistry Chemical Physics, 2015, 17, 18121-18130.	1.3	22
95	Separation of benzene from mixtures with water, methanol, ethanol, and acetone: highlighting hydrogen bonding and molecular clustering influences in CuBTC. Physical Chemistry Chemical Physics, 2015, 17, 20114-20124.	1.3	20
96	Design and development of a controlled pressure/temperature set-up forin situstudies ofÂsolidâ€“gas processes and reactions in a synchrotron X-ray powder diffraction station. Journal of Synchrotron Radiation, 2015, 22, 42-48.	1.0	11
97	Thermostructural behaviour of Niâ€“Cr materials: modelling of bulk and nanoparticle systems. Physical Chemistry Chemical Physics, 2015, 17, 15912-15920.	1.3	13
98	Underlying Adsorption Mechanisms of Water in Hydrophobic and Hydrophilic Zeolite Imidazolate Frameworks: ZIF-71 and ZIF-90. Journal of Physical Chemistry C, 2015, 119, 23774-23780.	1.5	30
99	On the performance of FAU and MFI zeolites for the adsorptive removal of a series of volatile organic compounds from air using molecular simulation. Physical Chemistry Chemical Physics, 2015, 17, 26451-26455.	1.3	23
100	Understanding and Exploiting Window Effects for Adsorption and Separations of Hydrocarbons. Journal of Physical Chemistry C, 2015, 119, 19236-19243.	1.5	13
101	Transferable force fields for adsorption of small gases in zeolites. Physical Chemistry Chemical Physics, 2015, 17, 24048-24055.	1.3	30
102	Understanding Nanopore Window Distortions in the Reversible Molecular Valve Zeolite RHO. Chemistry of Materials, 2015, 27, 5657-5667.	3.2	42
103	Electronic structure of porphyrin-based metalâ€“organic frameworks and their suitability for solar fuel production photocatalysis. Journal of Materials Chemistry A, 2015, 3, 23458-23465.	5.2	59
104	Entropic Separations of Mixtures of Aromatics by Selective Faceâ€toâ€Face Molecular Stacking in Oneâ€Dimensional Channels of Metalâ€“Organic Frameworks and Zeolites. ChemPhysChem, 2015, 16, 532-535.	1.0	17
105	Insights into the Adsorption of Water and Small Alcohols on the Open-Metal Sites of Cuâ€“BTC via Molecular Simulation. Journal of Physical Chemistry C, 2015, 119, 467-472.	1.5	20
106	Insights into the microscopic behaviour of nanoconfined water: host structure and thermal effects. CrystEngComm, 2015, 17, 412-421.	1.3	17
107	Atomic charges for modeling metalâ€“organic frameworks: Why and how. Journal of Solid State Chemistry, 2015, 223, 144-151.	1.4	47
108	Exploring new methods and materials for enantioselective separations and catalysis. Molecular Simulation, 2014, 40, 585-598.	0.9	21

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109	Ion Transport in Electrolytes for Dye-Sensitized Solar Cells: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry C, 2014, 118, 28448-28455.	1.5	14
110	Hydrogen bonding of water confined in zeolites and their zeolitic imidazolate framework counterparts. RSC Advances, 2014, 4, 29571.	1.7	18
111	Insights on the Anomalous Adsorption of Carbon Dioxide in LTA Zeolites. Journal of Physical Chemistry C, 2014, 118, 25460-25467.	1.5	45
112	Optimisation of the Fischerâ€“Tropsch process using zeolites for tail gas separation. Physical Chemistry Chemical Physics, 2014, 16, 5678.	1.3	12
113	Zeolite screening for the separation of gas mixtures containing SO₂, CO₂and CO. Physical Chemistry Chemical Physics, 2014, 16, 19884.	1.3	81
114	Effect of the Confinement and Presence of Cations on Hydrogen Bonding of Water in LTA-Type Zeolite. Journal of Physical Chemistry C, 2014, 118, 9056-9065.	1.5	25
115	Solubility of the Precombustion Gases CO₂, CH₄, CO, H₂, N₂, and H₂S in the Ionic Liquid [bmim][Tf₂N] from Monte Carlo Simulations. Journal of Physical Chemistry C, 2014, 118, 23599-23604.	1.5	67
116	Enantioselective adsorption of ibuprofen and lysine in metalâ€“organic frameworks. Chemical Communications, 2014, 50, 10849.	2.2	52
117	Enantiomeric Adsorption of Lactic Acid Mixtures in Achiral Zeolites. Journal of Physical Chemistry C, 2014, 118, 14991-14997.	1.5	3
118	Selective Separation of BTEX Mixtures Using Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2014, 118, 13126-13136.	1.5	28
119	Adsorption of hydrogen sulphide on Metal-Organic Frameworks. RSC Advances, 2013, 3, 14737.	1.7	49
120	High Adsorption Capacities and Two-Step Adsorption of Polar Adsorbates on Copperâ€“Benzene-1,3,5-tricarboxylate Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2013, 117, 18100-18111.	1.5	67
121	Adsorption in Metal-Organic Frameworks. , 2013, , 989-1006.		3
122	Water adsorption in hydrophilic zeolites: experiment and simulation. Physical Chemistry Chemical Physics, 2013, 15, 17374.	1.3	66
123	Strategies to Simultaneously Enhance the Hydrostability and the Alcoholâ€“Water Separation Behavior of Cu-BTC. Journal of Physical Chemistry C, 2013, 117, 20706-20714.	1.5	23
124	How ligands improve the hydrothermal stability and affect the adsorption in the IRMOF family. Physical Chemistry Chemical Physics, 2013, 15, 17696.	1.3	29
125	Toward a Transferable Set of Charges to Model Zeolitic Imidazolate Frameworks: Combined Experimentalâ€“Theoretical Research. Journal of Physical Chemistry C, 2013, 117, 466-471.	1.5	24
126	COKâ€16: A Cationâ€Exchanging Metalâ€“Organic Framework Hybrid. ChemPlusChem, 2013, 78, 402-406.	1.3	15

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127	Understanding Adsorption of Highly Polar Vapors on Mesoporous MIL-100(Cr) and MIL-101(Cr): Experiments and Molecular Simulations. Journal of Physical Chemistry C, 2013, 117, 7613-7622.	1.5	79
128	Molecular Mechanisms for Adsorption in Cu-BTC Metal Organic Framework. Journal of Physical Chemistry C, 2013, 117, 11357-11366.	1.5	81
129	Simulation Study of Structural Changes in Zeolite RHO. Journal of Physical Chemistry C, 2013, 117, 11592-11599.	1.5	23
130	Insights on the Molecular Mechanisms of Hydrogen Adsorption in Zeolites. Journal of Physical Chemistry C, 2013, 117, 14374-14380.	1.5	33
131	Understanding Hydrocarbon Adsorption in the UiO-66 Metalâ€“Organic Framework: Separation of (Un)saturated Linear, Branched, Cyclic Adsorbates, Including Stereoisomers. Journal of Physical Chemistry C, 2013, 117, 12567-12578.	1.5	69
132	Effect of the molecular interactions on the separation of nonpolar mixtures using Cu-BTC metalâ€“organic framework. Microporous and Mesoporous Materials, 2013, 165, 79-83.	2.2	13
133	Effect of Room-Temperature Ionic Liquids on CO₂ Separation by a Cu-BTC Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2013, 117, 20762-20768.	1.5	84
134	Adsorption of Polar Enantiomers in Achiral Zeolites. Journal of Physical Chemistry C, 2013, 117, 1524-1530.	1.5	12
135	Computerâ€Assisted Screening of Ordered Crystalline Nanoporous Adsorbents for Separation of Alkane Isomers. Angewandte Chemie - International Edition, 2012, 51, 11867-11871.	7.2	89
136	On the Mechanism Behind the Instability of Isoreticular Metalâ€“Organic Frameworks (IRMOFs) in Humid Environments. Chemistry - A European Journal, 2012, 18, 12260-12266.	1.7	66
137	Early stages in the degradation of metalâ€“organic frameworks in liquid water from first-principles molecular dynamics. Physical Chemistry Chemical Physics, 2012, 14, 7240.	1.3	52
138	Fick Diffusion Coefficients in Ternary Liquid Systems from Equilibrium Molecular Dynamics Simulations. Industrial & Engineering Chemistry Research, 2012, 51, 10247-10258.	1.8	79
139	Understanding Carbon Monoxide Capture Using Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2012, 116, 6655-6663.	1.5	62
140	Zeolite Force Fields and Experimental Siliceous Frameworks in a Comparative Infrared Study. Journal of Physical Chemistry C, 2012, 116, 25797-25805.	1.5	28
141	Functionalisation of MOF open metal sites with pendant amines for CO2 capture. Journal of Materials Chemistry, 2012, 22, 10155.	6.7	110
142	Understanding Gas-Induced Structural Deformation of ZIF-8. Journal of Physical Chemistry Letters, 2012, 3, 1159-1164.	2.1	143
143	Influence of force field parameters on computed diffusion coefficients of CO2 in LTA-type zeolite. Microporous and Mesoporous Materials, 2012, 158, 64-76.	2.2	12
144	Effect of air humidity on the removal of carbon tetrachloride from air using Cuâ€“BTC metalâ€“organic framework. Physical Chemistry Chemical Physics, 2011, 13, 11165.	1.3	40

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145	Molecular simulation investigation into the performance of Cuâ€"BTC metalâ€"organic frameworks for carbon dioxideâ€"methane separations. Physical Chemistry Chemical Physics, 2011, 13, 20453.	1.3	25
146	Predictive Model for Optimizing Guestâ€"Host Lennardâ€"Jones Interactions in Zeolites. Journal of Physical Chemistry C, 2011, 115, 10187-10195.	1.5	1
147	On the performance of Cu-BTC metal organic framework for carbon tetrachloride gas removal. Chemical Communications, 2011, 47, 508-510.	2.2	32
148	External Surface Adsorption on Silicalite-1 Zeolite Studied by Molecular Simulation. Journal of Physical Chemistry C, 2011, 115, 15355-15360.	1.5	18
149	Influence of the sodium and calcium non-framework cations on the adsorption of hexane isomers in zeolite BEA. Theoretical Chemistry Accounts, 2011, 128, 695-703.	0.5	6
150	A Simulation Study of Hydrogen in Metalâ€"Organic Frameworks. Adsorption Science and Technology, 2010, 28, 823-835.	1.5	14
151	Enantioselective Adsorption in Achiral Zeolites. Angewandte Chemie - International Edition, 2010, 49, 3010-3013.	7.2	36
152	On the application of chiral amplification via adsorption. Chemical Engineering Science, 2010, 65, 6478-6485.	1.9	6
153	Analysis of the ITQ-12 Zeolite Performance in Propaneâ^'Propylene Separations Using a Combination of Experiments and Molecular Simulations. Journal of Physical Chemistry C, 2010, 114, 14907-14914.	1.5	47
154	Performance of Chiral Zeolites for Enantiomeric Separation Revealed by Molecular Simulation. Journal of Physical Chemistry C, 2010, 114, 22207-22213.	1.5	34
155	Modeling Adsorption and Self-Diffusion of Methane in LTA Zeolites: The Influence of Framework Flexibility. Journal of Physical Chemistry C, 2010, 114, 15068-15074.	1.5	84
156	Effective Monte Carlo Scheme for Multicomponent Gas Adsorption and Enantioselectivity in Nanoporous Materials. Journal of Physical Chemistry Letters, 2010, 1, 2154-2158.	2.1	14
157	Enantioselective Adsorption Characteristics of Aluminum-Substituted MFI Zeolites. Chemistry of Materials, 2010, 22, 4591-4601.	3.2	15
158	Identification of Adsorption Sites in Cu-BTC by Experimentation and Molecular Simulation. Langmuir, 2009, 25, 1725-1731.	1.6	98
159	Adsorption and Diffusion of Water, Methanol, and Ethanol in All-Silica DD3R: Experiments and Simulation. Journal of Physical Chemistry C, 2009, 113, 14290-14301.	1.5	69
160	Molecular Simulation Study on the Separation of Xylene Isomers in MIL-47 Metalâ^'Organic Frameworks. Journal of Physical Chemistry C, 2009, 113, 20869-20874.	1.5	67
161	Evaluation of various water models for simulation of adsorption in hydrophobic zeolites. Molecular Simulation, 2009, 35, 1067-1076.	0.9	60
162	Low-coverage adsorption properties of the metalâ€"organic framework MIL-47 studied by pulse chromatography and Monte Carlo simulations. Physical Chemistry Chemical Physics, 2009, 11, 3515.	1.3	73

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