

Sofia Calero

List of Publications by Year in descending order

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216
papers

9,747
citations

30047

54
h-index

49868

87
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230
all docs

230
docs citations

230
times ranked

7314
citing authors

#	ARTICLE	IF	CITATIONS
1	RASPA: molecular simulation software for adsorption and diffusion in flexible nanoporous materials. <i>Molecular Simulation</i> , 2016, 42, 81-101.	0.9	1,266
2	United Atom Force Field for Alkanes in Nanoporous Materials. <i>Journal of Physical Chemistry B</i> , 2004, 108, 12301-12313.	1.2	314
3	Understanding the Role of Sodium during Adsorption: A Force Field for Alkanes in Sodium-Exchanged Faujasites. <i>Journal of the American Chemical Society</i> , 2004, 126, 11377-11386.	6.6	255
4	Computing the Heat of Adsorption using Molecular Simulations: The Effect of Strong Coulombic Interactions. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1107-1118.	2.3	202
5	Transferable Force Field for Carbon Dioxide Adsorption in Zeolites. <i>Journal of Physical Chemistry C</i> , 2009, 113, 8814-8820.	1.5	199
6	Entropy effects during sorption of alkanes in zeolites. <i>Chemical Society Reviews</i> , 2002, 31, 185-194.	18.7	193
7	Understanding Water Adsorption in Cu-BTC Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2008, 112, 15934-15939.	1.5	178
8	A computational study of CO ₂ , N ₂ , and CH ₄ adsorption in zeolites. <i>Adsorption</i> , 2007, 13, 469-476.	1.4	159
9	Force Field Parametrization through Fitting on Inflection Points in Isotherms. <i>Physical Review Letters</i> , 2004, 93, 088302.	2.9	144
10	Understanding Gas-Induced Structural Deformation of ZIF-8. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 1159-1164.	2.1	143
11	Selective sulfur dioxide adsorption on crystal defect sites on an isorecticular metal organic framework series. <i>Nature Communications</i> , 2017, 8, 14457.	5.8	133
12	iRASPA: GPU-accelerated visualization software for materials scientists. <i>Molecular Simulation</i> , 2018, 44, 653-676.	0.9	112
13	Functionalisation of MOF open metal sites with pendant amines for CO ₂ capture. <i>Journal of Materials Chemistry</i> , 2012, 22, 10155.	6.7	110
14	Investigation of entropy effects during sorption of mixtures of alkanes in MFI zeolite. <i>Chemical Engineering Journal</i> , 2002, 88, 81-94.	6.6	109
15	Molecular simulations for adsorption and separation of natural gas in IRMOF-1 and Cu-BTC metal-organic frameworks. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 7085.	1.3	104
16	Identification of Adsorption Sites in Cu-BTC by Experimentation and Molecular Simulation. <i>Langmuir</i> , 2009, 25, 1725-1731.	1.6	98
17	Simulating the Effect of Nonframework Cations on the Adsorption of Alkanes in MFI-type Zeolites. <i>Journal of Physical Chemistry B</i> , 2003, 107, 12088-12096.	1.2	95
18	Homochiral Metal-Organic Frameworks for Enantioselective Separations in Liquid Chromatography. <i>Journal of the American Chemical Society</i> , 2019, 141, 14306-14316.	6.6	93

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19	On the molecular mechanisms for the H ₂ /CO ₂ separation performance of zeolite imidazolate framework two-layered membranes. <i>Chemical Science</i> , 2017, 8, 325-333.	3.7	91
20	Incommensurate Diffusion in Confined Systems. <i>Physical Review Letters</i> , 2003, 90, 245901.	2.9	89
21	Computer-Assisted Screening of Ordered Crystalline Nanoporous Adsorbents for Separation of Alkane Isomers. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 11867-11871.	7.2	89
22	Modeling Adsorption and Self-Diffusion of Methane in LTA Zeolites: The Influence of Framework Flexibility. <i>Journal of Physical Chemistry C</i> , 2010, 114, 15068-15074.	1.5	84
23	Effect of Room-Temperature Ionic Liquids on CO ₂ Separation by a Cu-BTC Metal-Organic Framework. <i>Journal of Physical Chemistry C</i> , 2013, 117, 20762-20768.	1.5	84
24	Porphyrin-based metal-organic frameworks for solar fuel synthesis photocatalysis: band gap tuning via iron substitutions. <i>Journal of Materials Chemistry A</i> , 2017, 5, 11894-11904.	5.2	84
25	Molecular Mechanisms for Adsorption in Cu-BTC Metal Organic Framework. <i>Journal of Physical Chemistry C</i> , 2013, 117, 11357-11366.	1.5	81
26	Zeolite screening for the separation of gas mixtures containing SO ₂ , CO ₂ and CO. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 19884.	1.3	81
27	Looking at the "Water-in-Deep-Eutectic-Solvent" System: A Dilution Range for High Performance Eutectics. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 17565-17573.	3.2	80
28	Fick Diffusion Coefficients in Ternary Liquid Systems from Equilibrium Molecular Dynamics Simulations. <i>Industrial & Engineering Chemistry Research</i> , 2012, 51, 10247-10258.	1.8	79
29	Understanding Adsorption of Highly Polar Vapors on Mesoporous MIL-100(Cr) and MIL-101(Cr): Experiments and Molecular Simulations. <i>Journal of Physical Chemistry C</i> , 2013, 117, 7613-7622.	1.5	79
30	The Influence of Non-framework Sodium Cations on the Adsorption of Alkanes in MFI- and MOR-Type Zeolites. <i>Journal of Physical Chemistry B</i> , 2002, 106, 10659-10667.	1.2	74
31	Low-coverage adsorption properties of the metal-organic framework MIL-47 studied by pulse chromatography and Monte Carlo simulations. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 3515.	1.3	73
32	Influence of Cation Na/Ca Ratio on Adsorption in LTA 5A: A Systematic Molecular Simulation Study of Alkane Chain Length. <i>Journal of Physical Chemistry B</i> , 2006, 110, 23968-23976.	1.2	72
33	Diffusion of CH ₄ and CO ₂ in MFI, CHA and DDR zeolites. <i>Chemical Physics Letters</i> , 2006, 429, 219-224.	1.2	69
34	Adsorption and Diffusion of Water, Methanol, and Ethanol in All-Silica DD3R: Experiments and Simulation. <i>Journal of Physical Chemistry C</i> , 2009, 113, 14290-14301.	1.5	69
35	Understanding Hydrocarbon Adsorption in the UiO-66 Metal-Organic Framework: Separation of (Un)saturated Linear, Branched, Cyclic Adsorbates, Including Stereoisomers. <i>Journal of Physical Chemistry C</i> , 2013, 117, 12567-12578.	1.5	69
36	Understanding the Window Effect in Zeolite Catalysis. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 3624-3626.	7.2	68

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37	Molecular Simulation Study on the Separation of Xylene Isomers in MIL-47 Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2009, 113, 20869-20874.	1.5	67
38	High Adsorption Capacities and Two-Step Adsorption of Polar Adsorbates on Copper-Benzene-1,3,5-tricarboxylate Metal-Organic Framework. <i>Journal of Physical Chemistry C</i> , 2013, 117, 18100-18111.	1.5	67
39	Solubility of the Precombustion Gases CO ₂ , CH ₄ , CO, H ₂ , N ₂ , and H ₂ S in the Ionic Liquid [bmim][Tf ₂ N] from Monte Carlo Simulations. <i>Journal of Physical Chemistry C</i> , 2014, 118, 23599-23604.	1.5	67
40	On the Mechanism Behind the Instability of Isoreticular Metal-Organic Frameworks (IRMOFs) in Humid Environments. <i>Chemistry - A European Journal</i> , 2012, 18, 12260-12266.	1.7	66
41	Water adsorption in hydrophilic zeolites: experiment and simulation. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17374.	1.3	66
42	Challenges of modeling nanostructured materials for photocatalytic water splitting. <i>Chemical Society Reviews</i> , 2022, 51, 3794-3818.	18.7	64
43	Incorporating the Loading Dependence of the Maxwell-Stefan Diffusivity in the Modeling of CH ₄ and CO ₂ Permeation Across Zeolite Membranes. <i>Industrial & Engineering Chemistry Research</i> , 2007, 46, 2974-2986.	1.8	63
44	A New United Atom Force Field for Adsorption of Alkenes in Zeolites. <i>Journal of Physical Chemistry C</i> , 2008, 112, 2492-2498.	1.5	62
45	Understanding Carbon Monoxide Capture Using Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2012, 116, 6655-6663.	1.5	62
46	Discovery of an Optimal Porous Crystalline Material for the Capture of Chemical Warfare Agents. <i>Chemistry of Materials</i> , 2018, 30, 4571-4579.	3.2	62
47	Understanding cage effects in the n-alkane conversion on zeolites. <i>Journal of Catalysis</i> , 2006, 237, 278-290.	3.1	61
48	Modelling a Linker Mismatch Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 16012-16016.	7.2	61
49	Separation of linear, mono-methyl and di-methyl alkanes in the 5-7 carbon atom range by exploiting configurational entropy effects during sorption on silicalite-1. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 4390-4398.	1.3	60
50	Shape selectivity through entropy. <i>Journal of Catalysis</i> , 2003, 214, 88-99.	3.1	60
51	Evaluation of various water models for simulation of adsorption in hydrophobic zeolites. <i>Molecular Simulation</i> , 2009, 35, 1067-1076.	0.9	60
52	Electronic structure of porphyrin-based metal-organic frameworks and their suitability for solar fuel production photocatalysis. <i>Journal of Materials Chemistry A</i> , 2015, 3, 23458-23465.	5.2	59
53	Unraveling the Argon Adsorption Processes in MFI-Type Zeolite. <i>Journal of Physical Chemistry C</i> , 2008, 112, 9976-9979.	1.5	57
54	Tuning the separation properties of zeolitic imidazolate framework core-shell structures via post-synthetic modification. <i>Journal of Materials Chemistry A</i> , 2017, 5, 25601-25608.	5.2	56

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55	Understanding Zeolite Catalysis: Inverse Shape Selectivity Revised. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 2499-2502.	7.2	54
56	High-throughput screening of metal-organic frameworks for CO ₂ and CH ₄ separation in the presence of water. <i>Chemical Engineering Journal</i> , 2021, 403, 126392.	6.6	53
57	Early stages in the degradation of metal-organic frameworks in liquid water from first-principles molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 7240.	1.3	52
58	Enantioselective adsorption of ibuprofen and lysine in metal-organic frameworks. <i>Chemical Communications</i> , 2014, 50, 10849.	2.2	52
59	Configurational Entropy Effects during Sorption of Hexane Isomers in Silicalite. <i>Journal of Catalysis</i> , 2001, 202, 395-401.	3.1	51
60	Adsorption of hydrogen sulphide on Metal-Organic Frameworks. <i>RSC Advances</i> , 2013, 3, 14737.	1.7	49
61	Alkane hydrocracking: shape selectivity or kinetics?. <i>Journal of Catalysis</i> , 2004, 221, 241-251.	3.1	47
62	Analysis of the ITQ-12 Zeolite Performance in Propane-Propylene Separations Using a Combination of Experiments and Molecular Simulations. <i>Journal of Physical Chemistry C</i> , 2010, 114, 14907-14914.	1.5	47
63	Atomic charges for modeling metal-organic frameworks: Why and how. <i>Journal of Solid State Chemistry</i> , 2015, 223, 144-151.	1.4	47
64	Adsorption and Diffusion of Benzene in Mg-MOF-74 with Open Metal Sites. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 4686-4700.	4.0	46
65	Insights on the Anomalous Adsorption of Carbon Dioxide in LTA Zeolites. <i>Journal of Physical Chemistry C</i> , 2014, 118, 25460-25467.	1.5	45
66	A Computational Method To Characterize Framework Aluminum in Aluminosilicates. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 276-278.	7.2	44
67	Dynamically Corrected Transition State Theory Calculations of Self-Diffusion in Anisotropic Nanoporous Materials. <i>Journal of Physical Chemistry B</i> , 2006, 110, 3164-3172.	1.2	43
68	Acetylene Storage and Separation Using Metal-Organic Frameworks with Open Metal Sites. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 31499-31507.	4.0	43
69	Understanding Nanopore Window Distortions in the Reversible Molecular Valve Zeolite RHO. <i>Chemistry of Materials</i> , 2015, 27, 5657-5667.	3.2	42
70	Controlling Thermal Expansion: A Metal-Organic Frameworks Route. <i>Chemistry of Materials</i> , 2016, 28, 8296-8304.	3.2	42
71	Design, Parameterization, and Implementation of Atomic Force Fields for Adsorption in Nanoporous Materials. <i>Advanced Theory and Simulations</i> , 2019, 2, 1900135.	1.3	41
72	Effect of air humidity on the removal of carbon tetrachloride from air using Cu-BTC metal-organic framework. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 11165.	1.3	40

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73	Micelle Formation in Aqueous Solutions of Room Temperature Ionic Liquids: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2017, 121, 8348-8358.	1.2	39
74	Role of Ionic Liquid [EMIM] ⁺ [SCN] ⁻ in the Adsorption and Diffusion of Gases in Metal-Organic Frameworks. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 29694-29704.	4.0	38
75	Understanding Aluminum Location and Non-framework Ions Effects on Alkane Adsorption in Aluminosilicates: A Molecular Simulation Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 10419-10426.	1.5	37
76	Role of hydrogen bonding in the capture and storage of ammonia in zeolites. <i>Chemical Engineering Journal</i> , 2020, 387, 124062.	6.6	37
77	Olefin/Paraffin Separation in Open Metal Site Cu-BTC Metal-Organic Framework. <i>Journal of Physical Chemistry C</i> , 2017, 121, 3126-3132.	1.5	37
78	Enantioselective Adsorption in Achiral Zeolites. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 3010-3013.	7.2	36
79	Storage and Separation of Carbon Dioxide and Methane in Hydrated Covalent Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2016, 120, 23756-23762.	1.5	36
80	Molecular Sieves for the Separation of Hydrogen Isotopes. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 18833-18840.	4.0	36
81	Performance of Chiral Zeolites for Enantiomeric Separation Revealed by Molecular Simulation. <i>Journal of Physical Chemistry C</i> , 2010, 114, 22207-22213.	1.5	34
82	Insights on the Molecular Mechanisms of Hydrogen Adsorption in Zeolites. <i>Journal of Physical Chemistry C</i> , 2013, 117, 14374-14380.	1.5	33
83	The Si-Ge substitutional series in the chiral STW zeolite structure type. <i>Journal of Materials Chemistry A</i> , 2018, 6, 15110-15122.	5.2	33
84	A Simulation Study of Alkanes in Linde Type A Zeolites. <i>Adsorption Science and Technology</i> , 2007, 25, 417-427.	1.5	32
85	On the performance of Cu-BTC metal organic framework for carbon tetrachloride gas removal. <i>Chemical Communications</i> , 2011, 47, 508-510.	2.2	32
86	Molecular dynamics simulations of organohalide perovskite precursors: solvent effects in the formation of perovskite solar cells. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 22770-22777.	1.3	32
87	Shape-selective n-alkane hydroconversion at exterior zeolite surfaces. <i>Journal of Catalysis</i> , 2008, 256, 95-107.	3.1	31
88	Solubilities of CO ₂ , CH ₄ , C ₂ H ₆ , and SO ₂ in ionic liquids and Selexol from Monte Carlo simulations. <i>Journal of Computational Science</i> , 2016, 15, 74-80.	1.5	31
89	High-pressure liquid phase hydroconversion of heptane/nonane mixtures on Pt/H-Y zeolite catalyst. <i>Journal of Catalysis</i> , 2003, 220, 66-73.	3.1	30
90	Molecular path control in zeolite membranes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 12317-12320.	3.3	30

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91	Underlying Adsorption Mechanisms of Water in Hydrophobic and Hydrophilic Zeolite Imidazolate Frameworks: ZIF-71 and ZIF-90. <i>Journal of Physical Chemistry C</i> , 2015, 119, 23774-23780.	1.5	30
92	Transferable force fields for adsorption of small gases in zeolites. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 24048-24055.	1.3	30
93	Zeolites for CO ₂ â€“O ₂ Separation to Obtain CO ₂ -Neutral Fuels. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 20512-20520.	4.0	30
94	How ligands improve the hydrothermal stability and affect the adsorption in the IRMOF family. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17696.	1.3	29
95	Selective Adsorption of Water from Mixtures with 1-Alcohols by Exploitation of Molecular Packing Effects in CuBTC. <i>Journal of Physical Chemistry C</i> , 2015, 119, 3658-3666.	1.5	29
96	Quantum and Classical Molecular Dynamics of Ionic Liquid Electrolytes for Na/Liâ€“based Batteries: Molecular Origins of the Conductivity Behavior. <i>ChemPhysChem</i> , 2016, 17, 2473-2481.	1.0	29
97	Accurate Simulations of the Vaporâ€“Liquid Equilibrium of Important Organic Solvents and Other Diatomics. <i>Journal of Physical Chemistry B</i> , 1997, 101, 6763-6771.	1.2	28
98	The selectivity of n-hexane hydroconversion on MOR-, MAZ-, and FAU-type zeolites. <i>Journal of Catalysis</i> , 2004, 228, 121-129.	3.1	28
99	Zeolite Force Fields and Experimental Siliceous Frameworks in a Comparative Infrared Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 25797-25805.	1.5	28
100	Selective Separation of BTEX Mixtures Using Metalâ€“Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2014, 118, 13126-13136.	1.5	28
101	Ï€-Complexation for olefin/paraffin separation using aluminosilicates. <i>Chemical Engineering Journal</i> , 2020, 380, 122482.	6.6	28
102	Water adsorption in ideal and defective UiO-66 structures. <i>Microporous and Mesoporous Materials</i> , 2022, 330, 111555.	2.2	28
103	Description of alternative refrigerants with BACKONE equations. <i>Fluid Phase Equilibria</i> , 1998, 152, 1-22.	1.4	27
104	Comparing gas separation performance between all known zeolites and their zeolitic imidazolate framework counterparts. <i>Dalton Transactions</i> , 2016, 45, 216-225.	1.6	26
105	Efficient modelling of ion structure and dynamics in inorganic metal halide perovskites. <i>Journal of Materials Chemistry A</i> , 2020, 8, 11824-11836.	5.2	26
106	A Coarse-Graining Approach for the Proton Complex in Protonated Aluminosilicates. <i>Journal of Physical Chemistry B</i> , 2006, 110, 5838-5841.	1.2	25
107	Molecular simulation investigation into the performance of Cuâ€“BTC metalâ€“organic frameworks for carbon dioxideâ€“methane separations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20453.	1.3	25
108	Effect of the Confinement and Presence of Cations on Hydrogen Bonding of Water in LTA-Type Zeolite. <i>Journal of Physical Chemistry C</i> , 2014, 118, 9056-9065.	1.5	25

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109	Improving Olefin Purification Using Metal Organic Frameworks with Open Metal Sites. ACS Applied Materials & Interfaces, 2018, 10, 16911-16917.	4.0	25
110	EMIMBF ₄ in ternary liquid mixtures of water, dimethyl sulfoxide and acetonitrile as tri-solvent-in-salt electrolytes for high-performance supercapacitors operating at -70°C. Energy Storage Materials, 2021, 40, 368-385.	9.5	25
111	Toward a Transferable Set of Charges to Model Zeolitic Imidazolate Frameworks: Combined Experimental/Theoretical Research. Journal of Physical Chemistry C, 2013, 117, 466-471.	1.5	24
112	Adsorptive process design for the separation of hexane isomers using zeolites. Physical Chemistry Chemical Physics, 2017, 19, 5037-5042.	1.3	24
113	Strategies to Simultaneously Enhance the Hydrostability and the Alcohol/Water Separation Behavior of Cu-BTC. Journal of Physical Chemistry C, 2013, 117, 20706-20714.	1.5	23
114	Simulation Study of Structural Changes in Zeolite RHO. Journal of Physical Chemistry C, 2013, 117, 11592-11599.	1.5	23
115	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
116	Molecular Dynamics Analysis of Charge Transport in Ionic Liquid Electrolytes Containing Added Salt with Mono, Di, and Trivalent Metal Cations. ChemPhysChem, 2018, 19, 1665-1673.	1.0	23
117	Exploiting the π -bonding for the separation of benzene and cyclohexane in zeolites. Chemical Engineering Journal, 2020, 398, 125678.	6.6	23
118	Zeolites for the selective adsorption of sulfur hexafluoride. Physical Chemistry Chemical Physics, 2015, 17, 18121-18130.	1.3	22
119	Critical Role of Dynamic Flexibility in Ge-Containing Zeolites: Impact on Diffusion. Chemistry - A European Journal, 2016, 22, 10036-10043.	1.7	22
120	Transitioning from Ionic Liquids to Deep Eutectic Solvents. ACS Sustainable Chemistry and Engineering, 2022, 10, 1232-1245.	3.2	22
121	Exploring new methods and materials for enantioselective separations and catalysis. Molecular Simulation, 2014, 40, 585-598.	0.9	21
122	Liquid self-diffusion of H ₂ O 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
123	Phase equilibria of a square-well monomer-dimer mixture: Gibbs ensemble computer simulation and statistical associating fluid theory for potentials of variable range. Physical Review E, 1998, 57, 2035-2044.	0.8	20
124	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
125	Insights into the Adsorption of Water and Small Alcohols on the Open-Metal Sites of Cu-BTC via Molecular Simulation. Journal of Physical Chemistry C, 2015, 119, 467-472.	1.5	20
126	Adsorptive separation of ethane and ethylene using IsoReticular Metal-Organic Frameworks. Microporous and Mesoporous Materials, 2017, 248, 40-45.	2.2	20

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127	Adsorption equilibrium of nitrogen dioxide in porous materials. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4189-4199.	1.3	20
128	Identifying Zeolite Topologies for Storage and Release of Hydrogen. <i>Journal of Physical Chemistry C</i> , 2018, 122, 12485-12493.	1.5	20
129	Further Extending the Dilution Range of the "Solvent-in-DES" Regime upon the Replacement of Water by an Organic Solvent with Hydrogen Bond Capabilities. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 12120-12131.	3.2	20
130	Impact of the Nature of Exchangeable Cations on LTA-Type Zeolite Hydration. <i>Journal of Physical Chemistry C</i> , 2016, 120, 23254-23261.	1.5	19
131	External Surface Adsorption on Silicalite-1 Zeolite Studied by Molecular Simulation. <i>Journal of Physical Chemistry C</i> , 2011, 115, 15355-15360.	1.5	18
132	Hydrogen bonding of water confined in zeolites and their zeolitic imidazolate framework counterparts. <i>RSC Advances</i> , 2014, 4, 29571.	1.7	18
133	Adsorption of <i>n</i> -Alkanes in MFI and MEL: Quasi-Equilibrated Thermodesorption Combined with Molecular Simulations. <i>Journal of Physical Chemistry C</i> , 2016, 120, 25338-25350.	1.5	18
134	Potential of polarizable force fields for predicting the separation performance of small hydrocarbons in M-MOF-74. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 28848-28859.	1.3	18
135	Enhancing the Water Capacity in Zr-Based Metal-Organic Framework for Heat Pump and Atmospheric Water Generator Applications. <i>ACS Applied Nano Materials</i> , 2019, 2, 3050-3059.	2.4	18
136	Entropic Separations of Mixtures of Aromatics by Selective Face-to-Face Molecular Stacking in One-Dimensional Channels of Metal-Organic Frameworks and Zeolites. <i>ChemPhysChem</i> , 2015, 16, 532-535.	1.0	17
137	Insights into the microscopic behaviour of nanoconfined water: host structure and thermal effects. <i>CrystEngComm</i> , 2015, 17, 412-421.	1.3	17
138	Importance of Blocking Inaccessible Voids on Modeling Zeolite Adsorption: Revisited. <i>Journal of Physical Chemistry C</i> , 2017, 121, 4462-4470.	1.5	17
139	Gate-Opening Mechanism of Hydrophilic-Hydrophobic Metal-Organic Frameworks: Molecular Simulations and Quasi-Equilibrated Desorption. <i>Chemistry of Materials</i> , 2018, 30, 5116-5127.	3.2	17
140	Potential of CO ₂ capture from flue gases by physicochemical and biological methods: A comparative study. <i>Chemical Engineering Journal</i> , 2021, 417, 128020.	6.6	17
141	Carbon Dioxide Capture Enhanced by Pre-Adsorption of Water and Methanol in UiO-66. <i>Chemistry - A European Journal</i> , 2021, 27, 14653-14659.	1.7	17
142	Elucidating alkane adsorption in sodium-exchanged zeolites from molecular simulations to empirical equations. <i>Applied Surface Science</i> , 2005, 252, 716-722.	3.1	16
143	Evaluation of a New Force Field for Describing the Adsorption Behavior of Alkanes in Various Pure Silica Zeolites. <i>Journal of Physical Chemistry B</i> , 2006, 110, 20166-20171.	1.2	16
144	Highly Selective Zeolite Topologies for Flue Gas Separation. <i>Chemistry - A European Journal</i> , 2016, 22, 18705-18708.	1.7	16

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145	Effective Model for Olefin/Paraffin Separation using (Co, Fe, Mn, Ni)â€MOFâ€74. ChemistrySelect, 2017, 2, 665-672.	0.7	16
146	Ordering of <i>n</i> -Alkanes Adsorbed in the Micropores of AlPO ₄ -5: A Combined Molecular Simulations and Quasi-Equilibrated Thermodesorption Study. Journal of Physical Chemistry C, 2017, 121, 25292-25302.	1.5	16
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148	Improving Ammonia Production Using Zeolites. Journal of Physical Chemistry C, 2019, 123, 18475-18481.	1.5	16
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