Sofia Calero

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2171954/publications.pdf

Version: 2024-02-01

216 papers	9,747 citations	29994 54 h-index	49773 87 g-index
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. Molecular Simulation, 2016, 42, 81-101.	0.9	1,266
2	United Atom Force Field for Alkanes in Nanoporous Materials. Journal of Physical Chemistry B, 2004, 108, 12301-12313.	1.2	314
3	Understanding the Role of Sodium during Adsorption:Â A Force Field for Alkanes in Sodium-Exchanged Faujasites. Journal of the American Chemical Society, 2004, 126, 11377-11386.	6.6	255
4	Computing the Heat of Adsorption using Molecular Simulations: The Effect of Strong Coulombic Interactions. Journal of Chemical Theory and Computation, 2008, 4, 1107-1118.	2.3	202
5	Transferable Force Field for Carbon Dioxide Adsorption in Zeolites. Journal of Physical Chemistry C, 2009, 113, 8814-8820.	1.5	199
6	Entropy effects during sorption of alkanes in zeolites. Chemical Society Reviews, 2002, 31, 185-194.	18.7	193
7	Understanding Water Adsorption in Cuâ^'BTC Metalâ^'Organic Frameworks. Journal of Physical Chemistry C, 2008, 112, 15934-15939.	1.5	178
8	A computational study of CO2, N2, and CH4 adsorption in zeolites. Adsorption, 2007, 13, 469-476.	1.4	159
9	Force Field Parametrization through Fitting on Inflection Points in Isotherms. Physical Review Letters, 2004, 93, 088302.	2.9	144
10	Understanding Gas-Induced Structural Deformation of ZIF-8. Journal of Physical Chemistry Letters, 2012, 3, 1159-1164.	2.1	143
11	Selective sulfur dioxide adsorption on crystal defect sites on an isoreticular metal organic framework series. Nature Communications, 2017, 8, 14457.	5.8	133
12	iRASPA: GPU-accelerated visualization software for materials scientists. Molecular Simulation, 2018, 44, 653-676.	0.9	112
13	Functionalisation of MOF open metal sites with pendant amines for CO2 capture. Journal of Materials Chemistry, 2012, 22, 10155.	6.7	110
14	Investigation of entropy effects during sorption of mixtures of alkanes in MFI zeolite. Chemical Engineering Journal, 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. Physical Chemistry Chemical Physics, 2008, 10, 7085.	1.3	104
16	Identification of Adsorption Sites in Cu-BTC by Experimentation and Molecular Simulation. Langmuir, 2009, 25, 1725-1731.	1.6	98
17	Simulating the Effect of Nonframework Cations on the Adsorption of Alkanes in MFI-type Zeolites. Journal of Physical Chemistry B, 2003, 107, 12088-12096.	1.2	95
18	Homochiral Metalâ€“Organic Frameworks for Enantioselective Separations in Liquid Chromatography. Journal of the American Chemical Society, 2019, 141, 14306-14316.	6.6	93

#	Article	IF	Citations
19	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
20	Incommensurate Diffusion in Confined Systems. Physical Review Letters, 2003, 90, 245901.	2.9	89
21	Computerâ€Assisted Screening of Ordered Crystalline Nanoporous Adsorbents for Separation of Alkane Isomers. Angewandte Chemie - International Edition, 2012, 51, 11867-11871.	7.2	89
22	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
23	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
24	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
25	Molecular Mechanisms for Adsorption in Cu-BTC Metal Organic Framework. Journal of Physical Chemistry C, 2013, 117, 11357-11366.	1.5	81
26	Zeolite screening for the separation of gas mixtures containing SO₂, CO₂and CO. Physical Chemistry Chemical Physics, 2014, 16, 19884.	1.3	81
27	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
28	Fick Diffusion Coefficients in Ternary Liquid Systems from Equilibrium Molecular Dynamics Simulations. Industrial & Engineering Chemistry Research, 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. Journal of Physical Chemistry C, 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. Journal of Physical Chemistry B, 2002, 106, 10659-10667.	1.2	74
31	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
32	Influence of Cation Na/Ca Ratio on Adsorption in LTA 5A:Â A Systematic Molecular Simulation Study of Alkane Chain Length. Journal of Physical Chemistry B, 2006, 110, 23968-23976.	1.2	72
33	Diffusion of CH4 and CO2 in MFI, CHA and DDR zeolites. Chemical Physics Letters, 2006, 429, 219-224.	1.2	69
34	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
35	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
36	Understanding the Window Effect in Zeolite Catalysis. Angewandte Chemie - International Edition, 2003, 42, 3624-3626.	7.2	68

#	Article	IF	Citations
37	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
38	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
39	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
40	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
41	Water adsorption in hydrophilic zeolites: experiment and simulation. Physical Chemistry Chemical Physics, 2013, 15, 17374.	1.3	66
42	Challenges of modeling nanostructured materials for photocatalytic water splitting. Chemical Society Reviews, 2022, 51, 3794-3818.	18.7	64
43	Incorporating the Loading Dependence of the Maxwellâ˜Stefan Diffusivity in the Modeling of CH4and CO2Permeation Across Zeolite Membranes. Industrial & Engineering Chemistry Research, 2007, 46, 2974-2986.	1.8	63
44	A New United Atom Force Field for Adsorption of Alkenes in Zeolites. Journal of Physical Chemistry C, 2008, 112, 2492-2498.	1.5	62
45	Understanding Carbon Monoxide Capture Using Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2012, 116, 6655-6663.	1.5	62
46	Discovery of an Optimal Porous Crystalline Material for the Capture of Chemical Warfare Agents. Chemistry of Materials, 2018, 30, 4571-4579.	3.2	62
47	Understanding cage effects in the n-alkane conversion on zeolites. Journal of Catalysis, 2006, 237, 278-290.	3.1	61
48	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
49	Separation of linear, mono-methyl and di-methyl alkanes in the 5â€“7 carbon atom range by exploiting configurational entropy effects during sorption on silicalite-1. Physical Chemistry Chemical Physics, 2001, 3, 4390-4398.	1.3	60
50	Shape selectivity through entropy. Journal of Catalysis, 2003, 214, 88-99.	3.1	60
51	Evaluation of various water models for simulation of adsorption in hydrophobic zeolites. Molecular Simulation, 2009, 35, 1067-1076.	0.9	60
52	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
53	Unraveling the Argon Adsorption Processes in MFI-Type Zeolite. Journal of Physical Chemistry C, 2008, 112, 9976-9979.	1.5	57
54	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

#	Article	IF	Citations
55	Understanding Zeolite Catalysis: Inverse Shape Selectivity Revised. Angewandte Chemie - International Edition, 2002, 41, 2499-2502.	7.2	54
56	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
57	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
58	Enantioselective adsorption of ibuprofen and lysine in metalâ€“organic frameworks. Chemical Communications, 2014, 50, 10849.	2.2	52
59	Configurational Entropy Effects during Sorption of Hexane Isomers in Silicalite. Journal of Catalysis, 2001, 202, 395-401.	3.1	51
60	Adsorption of hydrogen sulphide on Metal-Organic Frameworks. RSC Advances, 2013, 3, 14737.	1.7	49
61	Alkane hydrocracking: shape selectivity or kinetics?. Journal of Catalysis, 2004, 221, 241-251.	3.1	47
62	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
63	Atomic charges for modeling metalâ€“organic frameworks: Why and how. Journal of Solid State Chemistry, 2015, 223, 144-151.	1.4	47
64	Adsorption and Diffusion of Benzene in Mg-MOF-74 with Open Metal Sites. ACS Applied Materials & Interfaces, 2019, 11, 4686-4700.	4.0	46
65	Insights on the Anomalous Adsorption of Carbon Dioxide in LTA Zeolites. Journal of Physical Chemistry C, 2014, 118, 25460-25467.	1.5	45
66	A Computational Method To Characterize Framework Aluminum in Aluminosilicates. Angewandte Chemie - International Edition, 2007, 46, 276-278.	7.2	44
67	Dynamically Corrected Transition State Theory Calculations of Self-Diffusion in Anisotropic Nanoporous Materials. Journal of Physical Chemistry B, 2006, 110, 3164-3172.	1.2	43
68	Acetylene Storage and Separation Using Metalâ€“Organic Frameworks with Open Metal Sites. ACS Applied Materials & Interfaces, 2019, 11, 31499-31507.	4.0	43
69	Understanding Nanopore Window Distortions in the Reversible Molecular Valve Zeolite RHO. Chemistry of Materials, 2015, 27, 5657-5667.	3.2	42
70	Controlling Thermal Expansion: A Metalâ€“Organic Frameworks Route. Chemistry of Materials, 2016, 28, 8296-8304.	3.2	42
71	Design, Parameterization, and Implementation of Atomic Force Fields for Adsorption in Nanoporous Materials. Advanced Theory and Simulations, 2019, 2, 1900135.	1.3	41
72	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

#	Article	IF	Citations
73	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
74	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
75	Understanding Aluminum Location and Non-framework Ions Effects on Alkane Adsorption in Aluminosilicates:â€‰ A Molecular Simulation Study. Journal of Physical Chemistry C, 2007, 111, 10419-10426.	1.5	37
76	Role of hydrogen bonding in the capture and storage of ammonia in zeolites. Chemical Engineering Journal, 2020, 387, 124062.	6.6	37
77	Olefin/Paraffin Separation in Open Metal Site Cu-BTC Metalâ€"Organic Framework. Journal of Physical Chemistry C, 2017, 121, 3126-3132.	1.5	37
78	Enantioselective Adsorption in Achiral Zeolites. Angewandte Chemie - International Edition, 2010, 49, 3010-3013.	7.2	36
79	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
80	Molecular Sieves for the Separation of Hydrogen Isotopes. ACS Applied Materials & Interfaces, 2019, 11, 18833-18840.	4.0	36
81	Performance of Chiral Zeolites for Enantiomeric Separation Revealed by Molecular Simulation. Journal of Physical Chemistry C, 2010, 114, 22207-22213.	1.5	34
82	Insights on the Molecular Mechanisms of Hydrogen Adsorption in Zeolites. Journal of Physical Chemistry C, 2013, 117, 14374-14380.	1.5	33
83	The Siâ€"Ge substitutional series in the chiral STW zeolite structure type. Journal of Materials Chemistry A, 2018, 6, 15110-15122.	5.2	33
84	A Simulation Study of Alkanes in Linde Type A Zeolites. Adsorption Science and Technology, 2007, 25, 417-427.	1.5	32
85	On the performance of Cu-BTC metal organic framework for carbon tetrachloride gas removal. Chemical Communications, 2011, 47, 508-510.	2.2	32
86	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
87	Shape-selective n-alkane hydroconversion at exterior zeolite surfaces. Journal of Catalysis, 2008, 256, 95-107.	3.1	31
88	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
89	High-pressure liquid phase hydroconversion of heptane/nonane mixtures on Pt/H-Y zeolite catalyst. Journal of Catalysis, 2003, 220, 66-73.	3.1	30
90	Molecular path control in zeolite membranes. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 12317-12320.	3.3	30

#	Article	IF	Citations
91	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
92	Transferable force fields for adsorption of small gases in zeolites. Physical Chemistry Chemical Physics, 2015, 17, 24048-24055.	1.3	30
93	Zeolites for CO₂â€“COâ€“O₂ Separation to Obtain CO₂-Neutral Fuels. ACS Applied Materials & Interfaces, 2018, 10, 20512-20520.	4.0	30
94	How ligands improve the hydrothermal stability and affect the adsorption in the IRMOF family. Physical Chemistry Chemical Physics, 2013, 15, 17696.	1.3	29
95	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
96	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
97	Accurate Simulations of the Vaporâ^'Liquid Equilibrium of Important Organic Solvents and Other Diatomics. Journal of Physical Chemistry B, 1997, 101, 6763-6771.	1.2	28
98	The selectivity of -hexane hydroconversion on MOR-, MAZ-, and FAU-type zeolites. Journal of Catalysis, 2004, 228, 121-129.	3.1	28
99	Zeolite Force Fields and Experimental Siliceous Frameworks in a Comparative Infrared Study. Journal of Physical Chemistry C, 2012, 116, 25797-25805.	1.5	28
100	Selective Separation of BTEX Mixtures Using Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2014, 118, 13126-13136.	1.5	28
101	Ï€-Complexation for olefin/paraffin separation using aluminosilicates. Chemical Engineering Journal, 2020, 380, 122482.	6.6	28
102	Water adsorption in ideal and defective UiO-66 structures. Microporous and Mesoporous Materials, 2022, 330, 111555.	2.2	28
103	Description of alternative refrigerants with BACKONE equations. Fluid Phase Equilibria, 1998, 152, 1-22.	1.4	27
104	Comparing gas separation performance between all known zeolites and their zeolitic imidazolate framework counterparts. Dalton Transactions, 2016, 45, 216-225.	1.6	26
105	Efficient modelling of ion structure and dynamics in inorganic metal halide perovskites. Journal of Materials Chemistry A, 2020, 8, 11824-11836.	5.2	26
106	A Coarse-Graining Approach for the Proton Complex in Protonated Aluminosilicates. Journal of Physical Chemistry B, 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. Physical Chemistry Chemical Physics, 2011, 13, 20453.	1.3	25
108	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

#	Article	IF	Citations
109	Improving Olefin Purification Using Metal Organic Frameworks with Open Metal Sites. ACS Applied Materials & Interfaces, 2018, 10, 16911-16917.	4.0	25
110	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
111	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
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 Alcoholâ€“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 Ionicâ€Liquid Electrolytes Containing Added Salt with Mono, Di, and Trivalent Metal Cations. ChemPhysChem, 2018, 19, 1665-1673.	1.0	23
117	Exploiting the Ï€-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 Geâ€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 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
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 Cuâ€“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

#	Article	IF	Citations
127	Adsorption equilibrium of nitrogen dioxide in porous materials. Physical Chemistry Chemical Physics, 2018, 20, 4189-4199.	1.3	20
128	Identifying Zeolite Topologies for Storage and Release of Hydrogen. Journal of Physical Chemistry C, 2018, 122, 12485-12493.	1.5	20
129	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
130	Impact of the Nature of Exchangeable Cations on LTA-Type Zeolite Hydration. Journal of Physical Chemistry C, 2016, 120, 23254-23261.	1.5	19
131	External Surface Adsorption on Silicalite-1 Zeolite Studied by Molecular Simulation. Journal of Physical Chemistry C, 2011, 115, 15355-15360.	1.5	18
132	Hydrogen bonding of water confined in zeolites and their zeolitic imidazolate framework counterparts. RSC Advances, 2014, 4, 29571.	1.7	18
133	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
134	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
135	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
136	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
137	Insights into the microscopic behaviour of nanoconfined water: host structure and thermal effects. CrystEngComm, 2015, 17, 412-421.	1.3	17
138	Importance of Blocking Inaccessible Voids on Modeling Zeolite Adsorption: Revisited. Journal of Physical Chemistry C, 2017, 121, 4462-4470.	1.5	17
139	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
140	Potential of CO2 capture from flue gases by physicochemical and biological methods: A comparative study. Chemical Engineering Journal, 2021, 417, 128020.	6.6	17
141	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
142	Elucidating alkane adsorption in sodium-exchanged zeolites from molecular simulations to empirical equations. Applied Surface Science, 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. Journal of Physical Chemistry B, 2006, 110, 20166-20171.	1.2	16
144	Highly Selective Zeolite Topologies for Flue Gas Separation. Chemistry - A European Journal, 2016, 22, 18705-18708.	1.7	16

#	Article	IF	Citations
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 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
147	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
148	Improving Ammonia Production Using Zeolites. Journal of Physical Chemistry C, 2019, 123, 18475-18481.	1.5	16
149	Dynamical properties and transport coefficients of Kihara linear fluids. Journal of Chemical Physics, 1997, 106, 4753-4767.	1.2	15
150	Enantioselective Adsorption Characteristics of Aluminum-Substituted MFI Zeolites. Chemistry of Materials, 2010, 22, 4591-4601.	3.2	15
151	COKâ€16: A Cationâ€Exchanging Metalâ€“Organic Framework Hybrid. ChemPlusChem, 2013, 78, 402-406.	1.3	15
152	Phase Transition Induced by Gas Adsorption in Metalâ€Organic Frameworks. Chemistry - A European Journal, 2018, 24, 8530-8534.	1.7	15
153	Nonequilibrium properties of linear polar Kihara fluids from molecular dynamics. Results for models and for liquid acetonitrile. Journal of Chemical Physics, 1997, 107, 2034-2045.	1.2	14
154	A Simulation Study of Hydrogen in Metalâ€“Organic Frameworks. Adsorption Science and Technology, 2010, 28, 823-835.	1.5	14
155	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
156	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
157	Aqueous Solutions of Ionic Liquids: Microscopic Assembly. ChemPhysChem, 2016, 17, 380-386.	1.0	14
158	Influence of Flexibility on the Separation of Chiral Isomers in STWâ€Type Zeolite. Chemistry - A European Journal, 2018, 24, 4121-4132.	1.7	14
159	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
160	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
161	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
162	Thermostructural behaviour of Niâ€“Cr materials: modelling of bulk and nanoparticle systems. Physical Chemistry Chemical Physics, 2015, 17, 15912-15920.	1.3	13

#	Article	IF	Citations
163	Understanding and Exploiting Window Effects for Adsorption and Separations of Hydrocarbons. Journal of Physical Chemistry C, 2015, 119, 19236-19243.	1.5	13
164	Intermediate states approach for adsorption studies in flexible metalâ€“organic frameworks. Physical Chemistry Chemical Physics, 2019, 21, 3294-3303.	1.3	13
165	Structure of liquids composed of shifted dipole linear molecules. Physical Review E, 2003, 68, 021201.	0.8	12
166	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
167	Adsorption of Polar Enantiomers in Achiral Zeolites. Journal of Physical Chemistry C, 2013, 117, 1524-1530.	1.5	12
168	Optimisation of the Fischerâ€“Tropsch process using zeolites for tail gas separation. Physical Chemistry Chemical Physics, 2014, 16, 5678.	1.3	12
169	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
170	Cadmiumâ€“BINOL Metalâ€“Organic Framework for the Separation of Alcohol Isomers. Chemistry - A European Journal, 2017, 23, 874-885.	1.7	12
171	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
172	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
173	Stepped Propane Adsorption in Pure-Silica ITW Zeolite. Langmuir, 2018, 34, 4774-4779.	1.6	10
174	Enhancing separation efficiency in European syngas industry by using zeolites. Catalysis Today, 2021, 362, 113-121.	2.2	10
175	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
176	Effect of lattice shrinking on the migration of water within zeolite LTA. Microporous and Mesoporous Materials, 2020, 293, 109808.	2.2	9
177	Separation of Amyl Alcohol Isomers in ZIFâ€77. ChemPhysChem, 2015, 16, 2735-2738.	1.0	8
178	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
179	Adsorption of Cyclohexane in Pure Silica Zeolites: Highâ€Throughput Computational Screening Validated by Experimental Data. ChemPhysChem, 2018, 19, 3364-3371.	1.0	8
180	Aqueous Coâ€Solvent in Zwitterionicâ€based Protic Ionic Liquids as Electrolytes in 2.0â€…V Supercapacitors. ChemSusChem, 2020, 13, 5983-5995.	3.6	8

#	Article	IF	Citations
181	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
182	A new and more direct test of Hubbard relations from molecular mass distribution influence on linear liquid dynamics. Journal of Chemical Physics, 1999, 111, 5434-5440.	1.2	7
183	Highlights of (bio-)chemical tools and visualization software for computational science. Current Opinion in Chemical Engineering, 2019, 23, 1-13.	3.8	7
184	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
185	OCEAN: An Algorithm to Predict the Separation of Biogas Using Zeolites. Industrial & Engineering Chemistry Research, 2020, 59, 7212-7223.	1.8	7
186	In Silico Screening of Zeolites for High-Pressure Hydrogen Drying. ACS Applied Materials & Interfaces, 2021, 13, 8383-8394.	4.0	7
187	Revisiting Vibrational Spectroscopy to Tackle the Chemistry of Zr₆O₈ Metal-Organic Framework Nodes. ACS Applied Materials & Interfaces, 2022, 14, 27040-27047.	4.0	7
188	On the application of chiral amplification via adsorption. Chemical Engineering Science, 2010, 65, 6478-6485.	1.9	6
189	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
190	Diffusion Patterns in Zeolite MFI: The Cation Effect. Journal of Physical Chemistry C, 2018, 122, 29274-29284.	1.5	6
191	Suitability of the Kihara Potential To Predict Molecular Spectra of Linear Polyatomic Liquids. Journal of Physical Chemistry B, 2000, 104, 5808-5815.	1.2	5
192	Classical Molecular Dynamics Simulation of Kappa Squared Factor in Resonance Energy Transfer for Linear Dipole Models. Molecular Simulation, 2003, 29, 519-525.	0.9	5
193	Influence of charge distribution on the thermophysical and dynamical properties of polar linear molecules. Journal of Chemical Physics, 2003, 118, 11079-11091.	1.2	5
194	Adsorption of Light Alcohols in a High Hydrophobic Metal Azolate Framework. Journal of Physical Chemistry C, 2019, 123, 23987-23994.	1.5	5
195	The role of hydrogen bonding in the dehydration of bioalcohols in hydrophobic pervaporation membranes. Journal of Molecular Liquids, 2021, 340, 117297.	2.3	5
196	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
197	Beschreibung alternativer KÃltemittel und ihrer Gemische mit BACKONE-Gleichungen. Chemie-Ingenieur-Technik, 2000, 72, 738-742.	0.4	4
198	Molecular simulation of adsorption of n-alkanes in Na-MFI zeolites. Determination of empirical expressions. Studies in Surface Science and Catalysis, 2005, , 1097-1104.	1.5	4

#	Article	IF	Citations
199	The vapour - liquid equilibrium ofn-alkanes. Journal of Physics Condensed Matter, 1996, 8, 9643-9648.	0.7	3
200	Monte Carlo simulations of symmetric and asymmetric angular model liquids. Journal of Chemical Physics, 2001, 114, 9075-9082.	1.2	3
201	Modelling of the Complex between a 15-Residue Peptide from mSos2 and the N-Terminal SH3 Domain of Grb2 by Molecular-Dynamics Simulation. Chemistry and Biodiversity, 2004, 1, 505-519.	1.0	3
202	Adsorption in Metal-Organic Frameworks. , 2013, , 989-1006.		3
203	Enantiomeric Adsorption of Lactic Acid Mixtures in Achiral Zeolites. Journal of Physical Chemistry C, 2014, 118, 14991-14997.	1.5	3
204	Effect of diol isomer/water mixtures on the stability of Zn-MOF-74. Dalton Transactions, 2021, 50, 1808-1815.	1.6	3
205	Modifying the hydrophobic nature of MAF-6. Separation and Purification Technology, 2021, 277, 119422.	3.9	3
206	Separation of Volatile Organic Compounds in TAMOF-1. ACS Applied Materials & Interfaces, 2022, 14, 30772-30785.	4.0	3
207	Can models of charged rods show features of undercooled liquids?. Journal of Molecular Liquids, 2007, 134, 136-141.	2.3	2
208	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
209	Computational Approaches to Zeolite-Based Adsorption Processes. Structure and Bonding, 2020, , 57-83.	1.0	2
210	A new insight on the structural changes of linear quadrupole liquids. Journal of Chemical Physics, 2005, 123, 184502.	1.2	1
211	Searching the Microscopic Features Responsible for an Undercooled Liquid Behavior in Charged Rods. AIP Conference Proceedings, 2006, , .	0.3	1
212	Predictive Model for Optimizing Guestâ€“Host Lennardâ€“Jones Interactions in Zeolites. Journal of Physical Chemistry C, 2011, 115, 10187-10195.	1.5	1
213	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
214	Using Aliphatic Alcohols to Tune Benzene Adsorption in MAFâ€6. Advanced Theory and Simulations, 2019, 2, 1900112.	1.3	1
215	On the design of models for an accurate description of the water â€“ hematite interface. Applied Surface Science, 2021, 560, 149884.	3.1	1
216	Thermostructural Characterization of Silicon Carbide Nanocomposite Materials via Molecular Dynamics Simulations. Advanced Composite Materials, 2022, 31, 485-504.	1.0	0