Sofia Calero

List of Publications by Citations

215 papers	7,532 citations	49 h-index	77 g-index
230 ext. papers	8,615 ext. citations	6.1 avg, IF	6.21 L-index

#	Paper	IF	Citations
215	RASPA: molecular simulation software for adsorption and diffusion in flexible nanoporous materials. *Molecular Simulation*, **2016**, 42, 81-101	2	807
214	United Atom Force Field for Alkanes in Nanoporous Materials. *Journal of Physical Chemistry B*, **2004**, 108, 12301-12313	3.4	282
213	Understanding the role of sodium during adsorption: a force field for alkanes in sodium-exchanged faujasites. *Journal of the American Chemical Society*, **2004**, 126, 11377-86	16.4	222
212	Entropy effects during sorption of alkanes in zeolites. *Chemical Society Reviews*, **2002**, 31, 185-94	58.5	174
211	Transferable Force Field for Carbon Dioxide Adsorption in Zeolites. *Journal of Physical Chemistry C*, **2009**, 113, 8814-8820	3.8	160
210	Understanding Water Adsorption in Cu-BTC Metal-Organic Frameworks. *Journal of Physical Chemistry C*, **2008**, 112, 15934-15939	3.8	159
209	Computing the Heat of Adsorption using Molecular Simulations: The Effect of Strong Coulombic Interactions. *Journal of Chemical Theory and Computation*, **2008**, 4, 1107-18	6.4	157
208	A computational study of CO2, N2, and CH4 adsorption in zeolites. *Adsorption*, **2007**, 13, 469-476	2.6	145
207	Force field parametrization through fitting on inflection points in isotherms. *Physical Review Letters* , **2004**, 93, 088302	7.4	136
206	Understanding Gas-Induced Structural Deformation of ZIF-8. *Journal of Physical Chemistry Letters*, **2012**, 3, 1159-64	6.4	117
205	Functionalisation of MOF open metal sites with pendant amines for CO2 capture. *Journal of Materials Chemistry*, **2012**, 22, 10155		105
204	Selective sulfur dioxide adsorption on crystal defect sites on an isoreticular metal organic framework series. *Nature Communications*, **2017**, 8, 14457	17.4	101
203	Investigation of entropy effects during sorption of mixtures of alkanes in MFI zeolite. *Chemical Engineering Journal*, **2002**, 88, 81-94	14.7	101
202	Molecular simulations for adsorption and separation of natural gas in IRMOF-1 and Cu-BTC metal-organic frameworks. *Physical Chemistry Chemical Physics*, **2008**, 10, 7085-91	3.6	98
201	Identification of adsorption sites in Cu-BTC by experimentation and molecular simulation. *Langmuir* , **2009**, 25, 1725-31	4	92
200	Simulating the Effect of Nonframework Cations on the Adsorption of Alkanes in MFI-type Zeolites. *Journal of Physical Chemistry B*, **2003**, 107, 12088-12096	3.4	86
199	Incommensurate diffusion in confined systems. *Physical Review Letters*, **2003**, 90, 245901	7.4	82

198	Computer-assisted screening of ordered crystalline nanoporous adsorbents for separation of alkane isomers. *Angewandte Chemie - International Edition*, **2012**, 51, 11867-71	16.4	81
197	Modeling Adsorption and Self-Diffusion of Methane in LTA Zeolites: The Influence of Framework Flexibility. *Journal of Physical Chemistry C*, **2010**, 114, 15068-15074	3.8	74
196	Effect of Room-Temperature Ionic Liquids on CO2 Separation by a Cu-BTC Metal□Organic Framework. *Journal of Physical Chemistry C*, **2013**, 117, 20762-20768	3.8	72
195	Low-coverage adsorption properties of the metal-organic framework MIL-47 studied by pulse chromatography and Monte Carlo simulations. *Physical Chemistry Chemical Physics*, **2009**, 11, 3515-21	3.6	69
194	On the molecular mechanisms for the H/CO separation performance of zeolite imidazolate framework two-layered membranes. *Chemical Science*, **2017**, 8, 325-333	9.4	67
193	Molecular Mechanisms for Adsorption in Cu-BTC Metal Organic Framework. *Journal of Physical Chemistry C*, **2013**, 117, 11357-11366	3.8	66
192	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	3.4	66
191	Fick Diffusion Coefficients in Ternary Liquid Systems from Equilibrium Molecular Dynamics Simulations. *Industrial & Engineering Chemistry Research*, **2012**, 51, 10247-10258	3.9	63
190	Influence of cation Na/Ca ratio on adsorption in LTA 5A: a systematic molecular simulation study of alkane chain length. *Journal of Physical Chemistry B*, **2006**, 110, 23968-76	3.4	62
189	iRASPA: GPU-accelerated visualization software for materials scientists. *Molecular Simulation*, **2018**, 44, 653-676	2	61
188	Zeolite screening for the separation of gas mixtures containing SO2, CO2 and CO. *Physical Chemistry Chemical Physics*, **2014**, 16, 19884-93	3.6	61
187	Adsorption and Diffusion of Water, Methanol, and Ethanol in All-Silica DD3R: Experiments and Simulation. *Journal of Physical Chemistry C*, **2009**, 113, 14290-14301	3.8	61
186	Diffusion of CH4 and CO2 in MFI, CHA and DDR zeolites. *Chemical Physics Letters*, **2006**, 429, 219-224	2.5	61
185	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	3.8	60
184	Incorporating the Loading Dependence of the Maxwell□Stefan Diffusivity in the Modeling of CH4 and CO2 Permeation Across Zeolite Membranes. *Industrial & Engineering Chemistry Research*, **2007**, 46, 2974-2986	3.9	60
183	High Adsorption Capacities and Two-Step Adsorption of Polar Adsorbates on Copper□Benzene-1,3,5-tricarboxylate Metal□Organic Framework. *Journal of Physical Chemistry C*, **2013**, 117, 18100-18111	3.8	59
182	Understanding the window effect in zeolite catalysis. *Angewandte Chemie - International Edition*, **2003**, 42, 3624-6	16.4	59
181	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	13	57

180	Molecular Simulation Study on the Separation of Xylene Isomers in MIL-47 Metal Organic Frameworks. *Journal of Physical Chemistry C*, **2009**, 113, 20869-20874	3.8	57
179	Homochiral Metal-Organic Frameworks for Enantioselective Separations in Liquid Chromatography. *Journal of the American Chemical Society*, **2019**, 141, 14306-14316	16.4	56
178	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	3.8	56
177	Understanding Hydrocarbon Adsorption in the UiO-66 Metal Organic Framework: Separation of (Un)saturated Linear, Branched, Cyclic Adsorbates, Including Stereoisomers. *Journal of Physical Chemistry C*, **2013**, 117, 12567-12578	3.8	56
176	Separation of linear, mono-methyl and di-methyl alkanes in the 5 carbon atom range by exploiting configurational entropy effects during sorption on silicalite-1. *Physical Chemistry Chemical Physics*, **2001**, 3, 4390-4398	3.6	56
175	On the mechanism behind the instability of isoreticular metal-organic frameworks (IRMOFs) in humid environments. *Chemistry - A European Journal*, **2012**, 18, 12260-6	4.8	55
174	A New United Atom Force Field for Adsorption of Alkenes in Zeolites. *Journal of Physical Chemistry C*, **2008**, 112, 2492-2498	3.8	55
173	Shape selectivity through entropy. *Journal of Catalysis*, **2003**, 214, 88-99	7.3	54
172	Evaluation of various water models for simulation of adsorption in hydrophobic zeolites. *Molecular Simulation*, **2009**, 35, 1067-1076	2	52
171	Understanding Carbon Monoxide Capture Using Metal Organic Frameworks. *Journal of Physical Chemistry C*, **2012**, 116, 6655-6663	3.8	51
170	Understanding cage effects in the n-alkane conversion on zeolites. *Journal of Catalysis*, **2006**, 237, 278-290	7.3	51
169	Understanding zeolite catalysis: inverse shape selectivity revised. *Angewandte Chemie - International Edition*, **2002**, 41, 2499-502	16.4	50
168	Looking at the Water-in-Deep-Eutectic-Solvent System: A Dilution Range for High Performance Eutectics. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 17565-17573	8.3	49
167	Water adsorption in hydrophilic zeolites: experiment and simulation. *Physical Chemistry Chemical Physics*, **2013**, 15, 17374-82	3.6	49
166	Electronic structure of porphyrin-based metal organic frameworks and their suitability for solar fuel production photocatalysis. *Journal of Materials Chemistry A*, **2015**, 3, 23458-23465	13	47
165	Modelling a Linker Mix-and-Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. *Angewandte Chemie - International Edition*, **2016**, 55, 16012-16016	16.4	47
164	Unraveling the Argon Adsorption Processes in MFI-Type Zeolite. *Journal of Physical Chemistry C*, **2008**, 112, 9976-9979	3.8	47
163	Configurational Entropy Effects during Sorption of Hexane Isomers in Silicalite. *Journal of Catalysis*, **2001**, 202, 395-401	7.3	47

162	Early stages in the degradation of metal-organic frameworks in liquid water from first-principles molecular dynamics. *Physical Chemistry Chemical Physics*, **2012**, 14, 7240-5	3.6	44
161	Discovery of an Optimal Porous Crystalline Material for the Capture of Chemical Warfare Agents. *Chemistry of Materials*, **2018**, 30, 4571-4579	9.6	43
160	Enantioselective adsorption of ibuprofen and lysine in metal-organic frameworks. *Chemical Communications*, **2014**, 50, 10849-52	5.8	43
159	Analysis of the ITQ-12 Zeolite Performance in Propane–Propylene Separations Using a Combination of Experiments and Molecular Simulations. *Journal of Physical Chemistry C*, **2010**, 114, 14907-14914	3.8	42
158	Adsorption of hydrogen sulphide on Metal-Organic Frameworks. *RSC Advances*, **2013**, 3, 14737	3.7	40
157	Tuning the separation properties of zeolitic imidazolate framework core–shell structures via post-synthetic modification. *Journal of Materials Chemistry A*, **2017**, 5, 25601-25608	13	40
156	Alkane hydrocracking: shape selectivity or kinetics?. *Journal of Catalysis*, **2004**, 221, 241-251	7.3	38
155	Insights on the Anomalous Adsorption of Carbon Dioxide in LTA Zeolites. *Journal of Physical Chemistry C*, **2014**, 118, 25460-25467	3.8	37
154	A computational method to characterize framework aluminum in aluminosilicates. *Angewandte Chemie - International Edition*, **2007**, 46, 276-8	16.4	37
153	Atomic charges for modeling metal–organic frameworks: Why and how. *Journal of Solid State Chemistry*, **2015**, 223, 144-151	3.3	36
152	Dynamically corrected transition state theory calculations of self-diffusion in anisotropic nanoporous materials. *Journal of Physical Chemistry B*, **2006**, 110, 3164-72	3.4	36
151	Understanding Nanopore Window Distortions in the Reversible Molecular Valve Zeolite RHO. *Chemistry of Materials*, **2015**, 27, 5657-5667	9.6	34
150	Controlling Thermal Expansion: A Metal-Organic Frameworks Route. *Chemistry of Materials*, **2016**, 28, 8296-8304	9.6	33
149	Understanding Aluminum Location and Non-framework Ions Effects on Alkane Adsorption in Aluminosilicates: A Molecular Simulation Study. *Journal of Physical Chemistry C*, **2007**, 111, 10419-10426	3.8	33
148	On the performance of Cu-BTC metal organic framework for carbon tetrachloride gas removal. *Chemical Communications*, **2011**, 47, 508-10	5.8	32
147	Micelle Formation in Aqueous Solutions of Room Temperature Ionic Liquids: A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2017**, 121, 8348-8358	3.4	31
146	Enantioselective adsorption in achiral zeolites. *Angewandte Chemie - International Edition*, **2010**, 49, 3010-3	16.4	31
145	Effect of air humidity on the removal of carbon tetrachloride from air using Cu-BTC metal-organic framework. *Physical Chemistry Chemical Physics*, **2011**, 13, 11165-74	3.6	30

144	Molecular path control in zeolite membranes. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 12317-20	11.5	30
143	Performance of Chiral Zeolites for Enantiomeric Separation Revealed by Molecular Simulation. *Journal of Physical Chemistry C*, **2010**, 114, 22207-22213	3.8	29
142	High-pressure liquid phase hydroconversion of heptane/nonane mixtures on Pt/H-Y zeolite catalyst. *Journal of Catalysis*, **2003**, 220, 66-73	7.3	29
141	Storage and Separation of Carbon Dioxide and Methane in Hydrated Covalent Organic Frameworks. *Journal of Physical Chemistry C*, **2016**, 120, 23756-23762	3.8	28
140	Adsorption and Diffusion of Benzene in Mg-MOF-74 with Open Metal Sites. *ACS Applied Materials & Interfaces*, **2019**, 11, 4686-4700	9.5	28
139	Design, Parameterization, and Implementation of Atomic Force Fields for Adsorption in Nanoporous Materials. *Advanced Theory and Simulations*, **2019**, 2, 1900135	3.5	27
138	Description of alternative refrigerants with BACKONE equations. *Fluid Phase Equilibria*, **1998**, 152, 1-22	2.5	27
137	Shape-selective n-alkane hydroconversion at exterior zeolite surfaces. *Journal of Catalysis*, **2008**, 256, 95-107	7.3	27
136	The selectivity of -hexane hydroconversion on MOR-, MAZ-, and FAU-type zeolites. *Journal of Catalysis*, **2004**, 228, 121-129	7.3	27
135	Olefin/Paraffin Separation in Open Metal Site Cu-BTC Metal□Organic Framework. *Journal of Physical Chemistry C*, **2017**, 121, 3126-3132	3.8	27
134	Zeolite Force Fields and Experimental Siliceous Frameworks in a Comparative Infrared Study. *Journal of Physical Chemistry C*, **2012**, 116, 25797-25805	3.8	26
133	Accurate Simulations of the Vapor□Liquid Equilibrium of Important Organic Solvents and Other Diatomics. *Journal of Physical Chemistry B*, **1997**, 101, 6763-6771	3.4	25
132	Solubilities of CO2, CH4, C2H6, and SO2 in ionic liquids and Selexol from Monte Carlo simulations. *Journal of Computational Science*, **2016**, 15, 74-80	3.4	24
131	Quantum and Classical Molecular Dynamics of Ionic Liquid Electrolytes for Na/Li-based Batteries: Molecular Origins of the Conductivity Behavior. *ChemPhysChem*, **2016**, 17, 2473-81	3.2	24
130	Molecular simulation investigation into the performance of Cu-BTC metal-organic frameworks for carbon dioxide-methane separations. *Physical Chemistry Chemical Physics*, **2011**, 13, 20453-60	3.6	24
129	High-throughput screening of metal □Organic frameworks for CO2 and CH4 separation in the presence of water. *Chemical Engineering Journal*, **2021**, 403, 126392	14.7	24
128	Molecular dynamics simulations of organohalide perovskite precursors: solvent effects in the formation of perovskite solar cells. *Physical Chemistry Chemical Physics*, **2015**, 17, 22770-7	3.6	23
127	Role of Ionic Liquid [EMIM][SCN] in the Adsorption and Diffusion of Gases in Metal-Organic Frameworks. *ACS Applied Materials & Interfaces*, **2018**, 10, 29694-29704	9.5	23

126	Acetylene Storage and Separation Using Metal-Organic Frameworks with Open Metal Sites. *ACS Applied Materials & Interfaces*, **2019**, 11, 31499-31507	9.5	23
125	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	3.8	23
124	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	3.8	23
123	A coarse-graining approach for the proton complex in protonated aluminosilicates. *Journal of Physical Chemistry B*, **2006**, 110, 5838-41	3.4	23
122	Transferable force fields for adsorption of small gases in zeolites. *Physical Chemistry Chemical Physics*, **2015**, 17, 24048-55	3.6	22
121	Selective Separation of BTEX Mixtures Using Metal□Organic Frameworks. *Journal of Physical Chemistry C*, **2014**, 118, 13126-13136	3.8	22
120	How ligands improve the hydrothermal stability and affect the adsorption in the IRMOF family. *Physical Chemistry Chemical Physics*, **2013**, 15, 17696-704	3.6	22
119	Insights on the Molecular Mechanisms of Hydrogen Adsorption in Zeolites. *Journal of Physical Chemistry C*, **2013**, 117, 14374-14380	3.8	22
118	A Simulation Study of Alkanes in Linde Type A Zeolites. *Adsorption Science and Technology*, **2007**, 25, 417-427	3.6	22
117	Comparing gas separation performance between all known zeolites and their zeolitic imidazolate framework counterparts. *Dalton Transactions*, **2016**, 45, 216-25	4.3	21
116	Strategies to Simultaneously Enhance the Hydrostability and the Alcohol□Water Separation Behavior of Cu-BTC. *Journal of Physical Chemistry C*, **2013**, 117, 20706-20714	3.8	21
115	Molecular Sieves for the Separation of Hydrogen Isotopes. *ACS Applied Materials & Interfaces*, **2019**, 11, 18833-18840	9.5	20
114	Improving Olefin Purification Using Metal Organic Frameworks with Open Metal Sites. *ACS Applied Materials & Interfaces*, **2018**, 10, 16911-16917	9.5	20
113	The Si□Ge substitutional series in the chiral STW zeolite structure type. *Journal of Materials Chemistry A*, **2018**, 6, 15110-15122	13	20
112	Toward a Transferable Set of Charges to Model Zeolitic Imidazolate Frameworks: Combined Experimental□Theoretical Research. *Journal of Physical Chemistry C*, **2013**, 117, 466-471	3.8	20
111	Zeolites for CO-CO-O Separation to Obtain CO-Neutral Fuels. *ACS Applied Materials & Interfaces*, **2018**, 10, 20512-20520	9.5	20
110	Critical Role of Dynamic Flexibility in Ge-Containing Zeolites: Impact on Diffusion. *Chemistry - A European Journal*, **2016**, 22, 10036-43	4.8	19
109	Adsorptive separation of ethane and ethylene using IsoReticular Metal-Organic Frameworks. *Microporous and Mesoporous Materials*, **2017**, 248, 40-45	5.3	18

108	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, 19605-12	3.6	18
107	Adsorptive process design for the separation of hexane isomers using zeolites. *Physical Chemistry Chemical Physics*, **2017**, 19, 5037-5042	3.6	17
106	Adsorption equilibrium of nitrogen dioxide in porous materials. *Physical Chemistry Chemical Physics*, **2018**, 20, 4189-4199	3.6	17
105	Adsorption of n-Alkanes in MFI and MEL: Quasi-Equilibrated Thermodesorption Combined with Molecular Simulations. *Journal of Physical Chemistry C*, **2016**, 120, 25338-25350	3.8	17
104	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	2.4	17
103	Zeolites for the selective adsorption of sulfur hexafluoride. *Physical Chemistry Chemical Physics*, **2015**, 17, 18121-30	3.6	16
102	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, 26451-5	3.6	16
101	Insights into the Adsorption of Water and Small Alcohols on the Open-Metal Sites of CuBTC via Molecular Simulation. *Journal of Physical Chemistry C*, **2015**, 119, 467-472	3.8	16
100	Insights into the microscopic behaviour of nanoconfined water: host structure and thermal effects. *CrystEngComm*, **2015**, 17, 412-421	3.3	16
99	Simulation Study of Structural Changes in Zeolite RHO. *Journal of Physical Chemistry C*, **2013**, 117, 11592-11599	3.8	16
98	Impact of the Nature of Exchangeable Cations on LTA-Type Zeolite Hydration. *Journal of Physical Chemistry C*, **2016**, 120, 23254-23261	3.8	16
97	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	3.8	15
96	Entropic separations of mixtures of aromatics by selective face-to-face molecular stacking in one-dimensional channels of metal-organic frameworks and zeolites. *ChemPhysChem*, **2015**, 16, 532-5	3.2	15
95	Hydrogen bonding of water confined in zeolites and their zeolitic imidazolate framework counterparts. *RSC Advances*, **2014**, 4, 29571	3.7	15
94	Exploring new methods and materials for enantioselective separations and catalysis. *Molecular Simulation*, **2014**, 40, 585-598	2	15
93	Enantioselective Adsorption Characteristics of Aluminum-Substituted MFI Zeolites. *Chemistry of Materials*, **2010**, 22, 4591-4601	9.6	15
92	Elucidating alkane adsorption in sodium-exchanged zeolites from molecular simulations to empirical equations. *Applied Surface Science*, **2005**, 252, 716-722	6.7	15
91	Effective Model for Olefin/Paraffin Separation using (Co, Fe, Mn, Ni)-MOF-74. *ChemistrySelect*, **2017**, 2, 665-672	1.8	14

90	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	3.8	14
89	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	3.2	14
88	Effective Monte Carlo Scheme for Multicomponent Gas Adsorption and Enantioselectivity in Nanoporous Materials. *Journal of Physical Chemistry Letters*, **2010**, 1, 2154-2158	6.4	14
87	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, 20114-24	3.6	13
86	Highly Selective Zeolite Topologies for Flue Gas Separation. *Chemistry - A European Journal*, **2016**, 22, 18705-18708	4.8	13
85	Computer-Assisted Screening of Ordered Crystalline Nanoporous Adsorbents for Separation of Alkane Isomers. *Angewandte Chemie*, **2012**, 124, 12037-12041	3.6	13
84	COK-16: A Cation-Exchanging Metal□Organic Framework Hybrid. *ChemPlusChem*, **2013**, 78, 402-406	2.8	13
83	External Surface Adsorption on Silicalite-1 Zeolite Studied by Molecular Simulation. *Journal of Physical Chemistry C*, **2011**, 115, 15355-15360	3.8	13
82	Role of hydrogen bonding in the capture and storage of ammonia in zeolites. *Chemical Engineering Journal*, **2020**, 387, 124062	14.7	13
81	Importance of Blocking Inaccessible Voids on Modeling Zeolite Adsorption: Revisited. *Journal of Physical Chemistry C*, **2017**, 121, 4462-4470	3.8	12
80	Ion Transport in Electrolytes for Dye-Sensitized Solar Cells: A Combined Experimental and Theoretical Study. *Journal of Physical Chemistry C*, **2014**, 118, 28448-28455	3.8	12
79	A Simulation Study of Hydrogen in Metal□Organic Frameworks. *Adsorption Science and Technology*, **2010**, 28, 823-835	3.6	12
78	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	3.9	12
77	Dynamical properties and transport coefficients of Kihara linear fluids. *Journal of Chemical Physics*, **1997**, 106, 4753-4767	3.9	12
76	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, 20166-71	3.4	12
75	□Complexation for olefin/paraffin separation using aluminosilicates. *Chemical Engineering Journal*, **2020**, 380, 122482	14.7	12
74	Thermostructural behaviour of Ni-Cr materials: modelling of bulk and nanoparticle systems. *Physical Chemistry Chemical Physics*, **2015**, 17, 15912-20	3.6	11
73	Further Extending the Dilution Range of the □olvent-in-DES□Regime upon the Replacement of Water by an Organic Solvent with Hydrogen Bond Capabilities. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 12120-12131	8.3	11

72	Aqueous Solutions of Ionic Liquids: Microscopic Assembly. *ChemPhysChem*, **2016**, 17, 380-6	3.2	11
71	Optimisation of the Fischer-Tropsch process using zeolites for tail gas separation. *Physical Chemistry Chemical Physics*, **2014**, 16, 5678-88	3.6	11
70	Influence of force field parameters on computed diffusion coefficients of CO2 in LTA-type zeolite. *Microporous and Mesoporous Materials*, **2012**, 158, 64-76	5.3	11
69	Adsorption of Polar Enantiomers in Achiral Zeolites. *Journal of Physical Chemistry C*, **2013**, 117, 1524-1530	4.8	11
68	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	3.6	11
67	Enhancing the Water Capacity in Zr-Based Metal–Organic Framework for Heat Pump and Atmospheric Water Generator Applications. *ACS Applied Nano Materials*, **2019**, 2, 3050-3059	5.6	10
66	Phase Transition Induced by Gas Adsorption in Metal-Organic Frameworks. *Chemistry - A European Journal*, **2018**, 24, 8530-8534	4.8	10
65	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	3.6	10
64	Stepped Propane Adsorption in Pure-Silica ITW Zeolite. *Langmuir*, **2018**, 34, 4774-4779	4	10
63	Modelling a Linker Mix-and-Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. *Angewandte Chemie*, **2016**, 128, 16246-16250	3.6	10
62	Gate-Opening Mechanism of Hydrophilic–Hydrophobic Metal–Organic Frameworks: Molecular Simulations and Quasi-Equilibrated Desorption. *Chemistry of Materials*, **2018**, 30, 5116-5127	9.6	10
61	Improving Ammonia Production Using Zeolites. *Journal of Physical Chemistry C*, **2019**, 123, 18475-18481	3.8	10
60	EMIMBF4 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	19.4	10
59	Design and development of a controlled pressure/temperature set-up for in situ studies of solid-gas processes and reactions in a synchrotron X-ray powder diffraction station. *Journal of Synchrotron Radiation*, **2015**, 22, 42-8	2.4	9
58	Understanding and Exploiting Window Effects for Adsorption and Separations of Hydrocarbons. *Journal of Physical Chemistry C*, **2015**, 119, 19236-19243	3.8	9
57	Efficient modelling of ion structure and dynamics in inorganic metal halide perovskites. *Journal of Materials Chemistry A*, **2020**, 8, 11824-11836	13	9
56	Influence of Flexibility on the Separation of Chiral Isomers in STW-Type Zeolite. *Chemistry - A European Journal*, **2018**, 24, 4121-4132	4.8	9
55	Effect of the molecular interactions on the separation of nonpolar mixtures using Cu-BTC metal–organic framework. *Microporous and Mesoporous Materials*, **2013**, 165, 79-83	5.3	9

54	Structure of liquids composed of shifted dipole linear molecules. *Physical Review E*, **2003**, 68, 021201	2.4	9
53	Computing bubble-points of CO2/CH4 gas mixtures in ionic liquids from Monte Carlo simulations. *Fluid Phase Equilibria*, **2016**, 418, 100-107	2.5	8
52	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	3.8	8
51	Separation of Amyl Alcohol Isomers in ZIF-77. *ChemPhysChem*, **2015**, 16, 2735-2738	3.2	8
50	Intermediate states approach for adsorption studies in flexible metal-organic frameworks. *Physical Chemistry Chemical Physics*, **2019**, 21, 3294-3303	3.6	7
49	Effect of Light Gases in the Ethane/Ethylene Separation Using Zeolitic Imidazolate Frameworks. *Journal of Physical Chemistry C*, **2018**, 122, 8637-8646	3.8	7
48	Cadmium-BINOL Metal-Organic Framework for the Separation of Alcohol Isomers. *Chemistry - A European Journal*, **2017**, 23, 874-885	4.8	7
47	Identifying Zeolite Topologies for Storage and Release of Hydrogen. *Journal of Physical Chemistry C* , **2018**, 122, 12485-12493	3.8	7
46	Exploiting the Ebonding for the separation of benzene and cyclohexane in zeolites. *Chemical Engineering Journal*, **2020**, 398, 125678	14.7	6
45	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	1.9	6
44	Enantioselective Adsorption in Achiral Zeolites. *Angewandte Chemie*, **2010**, 122, 3074-3077	3.6	6
43	On the application of chiral amplification via adsorption. *Chemical Engineering Science*, **2010**, 65, 6478-6485	4.1	6
42	Effect of lattice shrinking on the migration of water within zeolite LTA. *Microporous and Mesoporous Materials*, **2020**, 293, 109808	5.3	6
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	3.8	6
40	Classical Molecular Dynamics Simulation of Kappa Squared Factor in Resonance Energy Transfer for Linear Dipole Models. *Molecular Simulation*, **2003**, 29, 519-525	2	5
39	Suitability of the Kihara Potential To Predict Molecular Spectra of Linear Polyatomic Liquids. *Journal of Physical Chemistry B*, **2000**, 104, 5808-5815	3.4	5
38	Challenges of modeling nanostructured materials for photocatalytic water splitting.. *Chemical Society Reviews*, **2022**,	58.5	5
37	Understanding the Window Effect in Zeolite Catalysis. *Angewandte Chemie*, **2003**, 115, 3752-3754	3.6	4

36	Influence of charge distribution on the thermophysical and dynamical properties of polar linear molecules. *Journal of Chemical Physics*, **2003**, 118, 11079-11091	3.9	4
35	Molecular simulation of adsorption of n-alkanes in Na-MFI zeolites. Determination of empirical expressions. *Studies in Surface Science and Catalysis*, **2005**, 1097-1104	1.8	4
34	Beschreibung alternativer K□emittel und ihrer Gemische mit BACKONE-Gleichungen. *Chemie-Ingenieur-Technik*, **2000**, 72, 738-742	0.8	4
33	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	3.9	4
32	Aqueous Co-Solvent in Zwitterionic-based Protic Ionic Liquids as Electrolytes in 2.0 V Supercapacitors. *ChemSusChem*, **2020**, 13, 5983-5995	8.3	4
31	Adsorption of Cyclohexane in Pure Silica Zeolites: High-Throughput Computational Screening Validated by Experimental Data. *ChemPhysChem*, **2018**, 19, 3364-3371	3.2	4
30	Highlights of (bio-)chemical tools and visualization software for computational science. *Current Opinion in Chemical Engineering*, **2019**, 23, 1-13	5.4	3
29	Enantiomeric Adsorption of Lactic Acid Mixtures in Achiral Zeolites. *Journal of Physical Chemistry C*, **2014**, 118, 14991-14997	3.8	3
28	Adsorption in Metal-Organic Frameworks **2013**, 989-1006		3
27	The vapour - liquid equilibrium ofn-alkanes. *Journal of Physics Condensed Matter*, **1996**, 8, 9643-9648	1.8	3
26	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, 505-19	2.5	3
25	Monte Carlo simulations of symmetric and asymmetric angular model liquids. *Journal of Chemical Physics*, **2001**, 114, 9075-9082	3.9	3
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	9.5	3
23	Enhancing separation efficiency in European syngas industry by using zeolites. *Catalysis Today*, **2021**, 362, 113-121	5.3	3
22	Carbon Dioxide Capture Enhanced by Pre-Adsorption of Water and Methanol in UiO-66. *Chemistry - A European Journal*, **2021**, 27, 14653-14659	4.8	3
21	Adsorption of Light Alcohols in a High Hydrophobic Metal Azolate Framework. *Journal of Physical Chemistry C*, **2019**, 123, 23987-23994	3.8	2
20	A Computational Method To Characterize Framework Aluminum in Aluminosilicates. *Angewandte Chemie*, **2007**, 119, 280-282	3.6	2
19	Can models of charged rods show features of undercooled liquids?. *Journal of Molecular Liquids*, **2007**, 134, 136-141	6	2

18	Water adsorption in ideal and defective UiO-66 structures. *Microporous and Mesoporous Materials*, **2021**, 111555	5.3	2
17	Potential of CO2 capture from flue gases by physicochemical and biological methods: A comparative study. *Chemical Engineering Journal*, **2021**, 417, 128020	14.7	2
16	Diffusion Patterns in Zeolite MFI: The Cation Effect. *Journal of Physical Chemistry C*, **2018**, 122, 29274-29284	3.8	2
15	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	6.1	2
14	OCEAN: An Algorithm to Predict the Separation of Biogas Using Zeolites. *Industrial & Engineering Chemistry Research*, **2020**, 59, 7212-7223	3.9	1
13	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	3.6	1
12	Using Aliphatic Alcohols to Tune Benzene Adsorption in MAF-6. *Advanced Theory and Simulations*, **2019**, 2, 1900112	3.5	1
11	Predictive Model for Optimizing Guest□Host Lennard□Jones Interactions in Zeolites. *Journal of Physical Chemistry C*, **2011**, 115, 10187-10195	3.8	1
10	A new insight on the structural changes of linear quadrupole liquids. *Journal of Chemical Physics*, **2005**, 123, 184502	3.9	1
9	Transitioning from Ionic Liquids to Deep Eutectic Solvents. *ACS Sustainable Chemistry and Engineering*, **2022**, 10, 1232-1245	8.3	1
8	Frontispiece: Modelling a Linker Mix-and-Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. *Angewandte Chemie - International Edition*, **2016**, 55,	16.4	1
7	Effect of diol isomer/water mixtures on the stability of Zn-MOF-74. *Dalton Transactions*, **2021**, 50, 1808-1815	4.3	1
6	In Silico Screening of Zeolites for High-Pressure Hydrogen Drying. *ACS Applied Materials & Interfaces*, **2021**, 13, 8383-8394	9.5	1
5	The role of hydrogen bonding in the dehydration of bioalcohols in hydrophobic pervaporation membranes. *Journal of Molecular Liquids*, **2021**, 340, 117297	6	1
4	Modifying the hydrophobic nature of MAF-6. *Separation and Purification Technology*, **2021**, 277, 119422	8.3	1
3	Computational Approaches to Zeolite-Based Adsorption Processes. *Structure and Bonding*, **2020**, 57-83	0.9	0
2	On the design of models for an accurate description of the water □hematite interface. *Applied Surface Science*, **2021**, 560, 149884	6.7	0
1	Thermostructural Characterization of Silicon Carbide Nanocomposite Materials via Molecular Dynamics Simulations. *Advanced Composite Materials*,1-20	2.8	