David Dubbeldam

List of Publications by Year
in descending order

143 papers	9,198 citations	46984 47 h-index	43868 91 g-index
156 all docs	156 docs citations	156 times ranked	6352 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	Understanding Inflections and Steps in Carbon Dioxide Adsorption Isotherms in Metal-Organic Frameworks. Journal of the American Chemical Society, 2008, 130, 406-407.	6.6	485
3	On the inner workings of Monte Carlo codes. Molecular Simulation, 2013, 39, 1253-1292.	0.9	325
4	United Atom Force Field for Alkanes in Nanoporous Materials. Journal of Physical Chemistry B, 2004, 108, 12301-12313.	1.2	314
5	Exceptional Negative Thermal Expansion in Isoreticular Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2007, 46, 4496-4499.	7.2	289
6	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
7	Heats of Adsorption for Seven Gases in Three Metalâ”Organic Frameworks: Systematic Comparison of Experiment and Simulation. Langmuir, 2009, 25, 7383-7388.	1.6	212
8	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
9	Transferable Force Field for Carbon Dioxide Adsorption in Zeolites. Journal of Physical Chemistry C, 2009, 113, 8814-8820.	1.5	199
10	Recent developments in the molecular modeling of diffusion in nanoporous materials. Molecular Simulation, 2007, 33, 305-325.	0.9	166
11	Mechanical Properties in Metalâ€“Organic Frameworks: Emerging Opportunities and Challenges for Device Functionality and Technological Applications. Advanced Materials, 2018, 30, e1704124.	11.1	165
12	A computational study of CO2, N2, and CH4 adsorption in zeolites. Adsorption, 2007, 13, 469-476.	1.4	159
13	Feasibility of zeolitic imidazolate framework membranes for clean energy applications. Energy and Environmental Science, 2012, 5, 7637.	15.6	154
14	Force Field Parametrization through Fitting on Inflection Points in Isotherms. Physical Review Letters, 2004, 93, 088302.	2.9	144
15	Molecular simulation of loading-dependent diffusion in nanoporous materials using extended dynamically corrected transition state theory. Journal of Chemical Physics, 2005, 122, 224712.	1.2	142
16	Molecular simulation of adsorption sites of light gases in the metal-organic framework IRMOF-1. Fluid Phase Equilibria, 2007, 261, 152-161.	1.4	129
17	Separation and Molecular-Level Segregation of Complex Alkane Mixtures in Metalâ”Organic Frameworks. Journal of the American Chemical Society, 2008, 130, 10884-10885.	6.6	116
18	iRASPA: GPU-accelerated visualization software for materials scientists. Molecular Simulation, 2018, 44, 653-676.	0.9	112

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19	Molecular Simulation of Loading Dependent Slow Diffusion in Confined Systems. Physical Review Letters, 2004, 93, 248301.	2.9	108
20	Understanding Diffusion in Nanoporous Materials. Physical Review Letters, 2006, 96, 044501.	2.9	104
21	Molecular-level Insight into Unusual Low Pressure CO₂ Affinity in Pillared Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2013, 135, 7172-7180.	6.6	100
22	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
23	Separating Xylene Isomers by Commensurate Stacking of pâ€Xylene within Channels of MAFâ€X8. Angewandte Chemie - International Edition, 2014, 53, 7774-7778.	7.2	93
24	Incommensurate Diffusion in Confined Systems. Physical Review Letters, 2003, 90, 245901.	2.9	89
25	Computerâ€Assisted Screening of Ordered Crystalline Nanoporous Adsorbents for Separation of Alkane Isomers. Angewandte Chemie - International Edition, 2012, 51, 11867-11871.	7.2	89
26	Polarizable Force Fields for CO₂ and CH₄ Adsorption in M-MOF-74. Journal of Physical Chemistry C, 2017, 121, 4659-4673.	1.5	87
27	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
28	Computer Simulation of Incommensurate Diffusion in Zeolites:Â Understanding Window Effects. Journal of Physical Chemistry B, 2003, 107, 12138-12152.	1.2	83
29	A new perspective on the order-nalgorithm for computing correlation functions. Molecular Simulation, 2009, 35, 1084-1097.	0.9	82
30	Self-Diffusion Studies in CuBTC by PFG NMR and MD Simulations. Journal of Physical Chemistry C, 2010, 114, 10527-10534.	1.5	82
31	Molecular Mechanisms for Adsorption in Cu-BTC Metal Organic Framework. Journal of Physical Chemistry C, 2013, 117, 11357-11366.	1.5	81
32	The distributed ASCI Supercomputer project. Operating Systems Review (ACM), 2000, 34, 76-96.	1.5	80
33	Loading Dependence of the Diffusion Coefficient of Methane in Nanoporous Materials. Journal of Physical Chemistry B, 2006, 110, 22754-22772.	1.2	80
34	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
35	Method for Analyzing Structural Changes of Flexible Metalâ^'Organic Frameworks Induced by Adsorbates. Journal of Physical Chemistry C, 2009, 113, 19317-19327.	1.5	71
36	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

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37	Understanding the Window Effect in Zeolite Catalysis. Angewandte Chemie - International Edition, 2003, 42, 3624-3626.	7.2	68
38	Strategies for Characterization of Large-Pore Metal-Organic Frameworks by Combined Experimental and Computational Methods. Chemistry of Materials, 2009, 21, 4768-4777.	3.2	68
39	Understanding cage effects in the n-alkane conversion on zeolites. Journal of Catalysis, 2006, 237, 278-290.	3.1	61
40	Evaluation of various water models for simulation of adsorption in hydrophobic zeolites. Molecular Simulation, 2009, 35, 1067-1076.	0.9	60
41	A Comparison of Advanced Monte Carlo Methods for Open Systems: CFCMC vs CBMC. Journal of Chemical Theory and Computation, 2014, 10, 942-952.	2.3	60
42	Self-Diffusion of Chain Molecules in the Metalâ€“Organic Framework IRMOF-1: Simulation and Experiment. Journal of Physical Chemistry Letters, 2012, 3, 930-933.	2.1	59
43	Unraveling the Argon Adsorption Processes in MFI-Type Zeolite. Journal of Physical Chemistry C, 2008, 112, 9976-9979.	1.5	57
44	In situ visualization of loading-dependent water effects in a stable metalâ€“organic framework. Nature Chemistry, 2020, 12, 186-192.	6.6	53
45	Enantioselective adsorption of ibuprofen and lysine in metalâ€“organic frameworks. Chemical Communications, 2014, 50, 10849.	2.2	52
46	Adsorption of hydrogen sulphide on Metal-Organic Frameworks. RSC Advances, 2013, 3, 14737.	1.7	49
47	On flexible force fields for metalâ€“organic frameworks: Recent developments and future prospects. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1363.	6.2	49
48	Molecular Understanding of Diffusion in Confinement. Physical Review Letters, 2005, 95, 164505.	2.9	48
49	Negative Thermal Expansion Design Strategies in a Diverse Series of Metalâ€“Organic Frameworks. Advanced Functional Materials, 2019, 29, 1904669.	7.8	48
50	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
51	Direct Free Energy Calculation in the Continuous Fractional Component Gibbs Ensemble. Journal of Chemical Theory and Computation, 2016, 12, 1481-1490.	2.3	47
52	Entropic Separation of Styrene/Ethylbenzene Mixtures by Exploitation of Subtle Differences in Molecular Configurations in Ordered Crystalline Nanoporous Adsorbents. Langmuir, 2015, 31, 3771-3778.	1.6	46
53	A Computational Method To Characterize Framework Aluminum in Aluminosilicates. Angewandte Chemie - International Edition, 2007, 46, 276-278.	7.2	44
54	Product shape selectivity of MFI-type, MEL-type, and BEA-type zeolites in the catalytic hydroconversion of heptane. Journal of Catalysis, 2017, 353, 54-62.	3.1	44

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55	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
56	Understanding Nanopore Window Distortions in the Reversible Molecular Valve Zeolite RHO. Chemistry of Materials, 2015, 27, 5657-5667.	3.2	42
57	Controlling Thermal Expansion: A Metalâ€“Organic Frameworks Route. Chemistry of Materials, 2016, 28, 8296-8304.	3.2	42
58	Behavior of the Enthalpy of Adsorption in Nanoporous Materials Close to Saturation Conditions. Journal of Chemical Theory and Computation, 2017, 13, 3326-3339.	2.3	41
59	Design, Parameterization, and Implementation of Atomic Force Fields for Adsorption in Nanoporous Materials. Advanced Theory and Simulations, 2019, 2, 1900135.	1.3	41
60	Elucidating steric effects on enantioselective epoxidation catalyzed by (salen)Mn in metal-organic frameworks. Journal of Molecular Catalysis A, 2011, 334, 89-97.	4.8	40
61	Absorption Refrigeration Cycles with Ammoniaâ€“Ionic Liquid Working Pairs Studied by Molecular Simulation. Industrial & Engineering Chemistry Research, 2018, 57, 5442-5452.	1.8	39
62	Recent advances in the continuous fractional component Monte Carlo methodology. Molecular Simulation, 2021, 47, 804-823.	0.9	38
63	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
64	Understanding DABCO Nanorotor Dynamics in Isostructural Metalâ€“Organic Frameworks. Journal of Physical Chemistry Letters, 2015, 6, 812-816.	2.1	37
65	Efficient Application of Continuous Fractional Component Monte Carlo in the Reaction Ensemble. Journal of Chemical Theory and Computation, 2017, 13, 4452-4466.	2.3	37
66	Enantioselective Adsorption in Achiral Zeolites. Angewandte Chemie - International Edition, 2010, 49, 3010-3013.	7.2	36
67	Prediction of adsorption isotherms from breakthrough curves. Microporous and Mesoporous Materials, 2019, 277, 237-244.	2.2	36
68	Synthesis of Chiral MOFâ€74 Frameworks by Postâ€Synthetic Modification by Using an Amino Acid. Chemistry - A European Journal, 2020, 26, 13957-13965.	1.7	35
69	Performance of Chiral Zeolites for Enantiomeric Separation Revealed by Molecular Simulation. Journal of Physical Chemistry C, 2010, 114, 22207-22213.	1.5	34
70	A Simulation Study of Alkanes in Linde Type A Zeolites. Adsorption Science and Technology, 2007, 25, 417-427.	1.5	32
71	Brick-CFCMC: Open Source Software for Monte Carlo Simulations of Phase and Reaction Equilibria Using the Continuous Fractional Component Method. Journal of Chemical Information and Modeling, 2020, 60, 2678-2682.	2.5	32
72	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

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73	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
74	Simulating the Reactions of CO2 in Aqueous Monoethanolamine Solution by Reaction Ensemble Monte Carlo Using the Continuous Fractional Component Method. Journal of Chemical Theory and Computation, 2015, 11, 2661-2669.	2.3	30
75	Solubility of sulfur compounds in commercial physical solvents and an ionic liquid from Monte Carlo simulations. Fluid Phase Equilibria, 2017, 433, 50-55.	1.4	29
76	Polarizable Force Field for CO₂ in M-MOF-74 Derived from Quantum Mechanics. Journal of Physical Chemistry C, 2018, 122, 24488-24498.	1.5	29
77	Waterâ€“Ethanol and Methanolâ€“Ethanol Separations Using in Situ Confined Polymer Chains in a Metalâ€“Organic Framework. ACS Applied Materials & Interfaces, 2019, 11, 41383-41393.	4.0	29
78	The selectivity of -hexane hydroconversion on MOR-, MAZ-, and FAU-type zeolites. Journal of Catalysis, 2004, 228, 121-129.	3.1	28
79	Zeolite Force Fields and Experimental Siliceous Frameworks in a Comparative Infrared Study. Journal of Physical Chemistry C, 2012, 116, 25797-25805.	1.5	28
80	Computation of partial molar properties using continuous fractional component Monte Carlo. Molecular Physics, 2018, 116, 3331-3344.	0.8	28
81	Exploiting Largeâ€Pore Metalâ€“Organic Frameworks for Separations through Entropic Molecular Mechanisms. ChemPhysChem, 2015, 16, 2046-2067.	1.0	27
82	Elucidating the Variable-Temperature Mechanical Properties of a Negative Thermal Expansion Metalâ€“Organic Framework. ACS Applied Materials & Interfaces, 2018, 10, 21079-21083.	4.0	27
83	On the Inflection in the Concentration Dependence of the Maxwellâ^'Stefan Diffusivity of CF4 in MFI Zeolite. Journal of Physical Chemistry B, 2004, 108, 14820-14822.	1.2	26
84	Solubility of Natural Gas Species in Ionic Liquids and Commercial Solvents: Experiments and Monte Carlo Simulations. Journal of Chemical & Engineering Data, 2015, 60, 3039-3045.	1.0	26
85	Efficient Separation of Ethanolâ€“Methanol and Ethanolâ€“Water Mixtures Using ZIF-8 Supported on a Hierarchical Porous Mixed-Oxide Substrate. ACS Applied Materials & Interfaces, 2019, 11, 21126-21136.	4.0	26
86	A Coarse-Graining Approach for the Proton Complex in Protonated Aluminosilicates. Journal of Physical Chemistry B, 2006, 110, 5838-5841.	1.2	25
87	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
88	Investigating polarization effects of CO2 adsorption in MgMOF-74. Journal of Computational Science, 2016, 15, 86-94.	1.5	25
89	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
90	Simulation Study of Structural Changes in Zeolite RHO. Journal of Physical Chemistry C, 2013, 117, 11592-11599.	1.5	23

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91	Exploring new methods and materials for enantioselective separations and catalysis. Molecular Simulation, 2014, 40, 585-598.	0.9	21
92	Computation of the Heat and Entropy of Adsorption in Proximity of Inflection Points. Journal of Physical Chemistry C, 2016, 120, 1727-1738.	1.5	21
93	Computation of thermodynamic properties in the continuous fractional component Monte Carlo Gibbs ensemble. Molecular Simulation, 2017, 43, 189-195.	0.9	20
94	Adsorption equilibrium of nitrogen dioxide in porous materials. Physical Chemistry Chemical Physics, 2018, 20, 4189-4199.	1.3	20
95	External Surface Adsorption on Silicalite-1 Zeolite Studied by Molecular Simulation. Journal of Physical Chemistry C, 2011, 115, 15355-15360.	1.5	18
96	Optimization of Particle Transfers in the Gibbs Ensemble for Systems with Strong and Directional Interactions Using CBMC, CFCMC, and CB/CFCMC. Journal of Physical Chemistry C, 2016, 120, 9148-9159.	1.5	18
97	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
98	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
99	Chemical potentials of water, methanol, carbon dioxide and hydrogen sulphide at low temperatures using continuous fractional component Gibbs ensemble Monte Carlo. Molecular Simulation, 2018, 44, 405-414.	0.9	17
100	Effect of truncating electrostatic interactions on predicting thermodynamic properties of waterâ€“methanol systems. Molecular Simulation, 2019, 45, 336-350.	0.9	17
101	Elucidating alkane adsorption in sodium-exchanged zeolites from molecular simulations to empirical equations. Applied Surface Science, 2005, 252, 716-722.	3.1	16
102	Distance and angular holonomic constraints in molecular simulations. Journal of Chemical Physics, 2010, 133, 034114.	1.2	16
103	Effective Model for Olefin/Paraffin Separation using (Co, Fe, Mn, Ni)â€MOFâ€74. ChemistrySelect, 2017, 2, 665-672.	0.7	16
104	Improving Ammonia Production Using Zeolites. Journal of Physical Chemistry C, 2019, 123, 18475-18481.	1.5	16
105	Effects of Framework Flexibility on the Adsorption and Diffusion of Aromatics in MFI-Type Zeolites. Journal of Physical Chemistry C, 2020, 124, 24488-24499.	1.5	16
106	Enantioselective Adsorption Characteristics of Aluminum-Substituted MFI Zeolites. Chemistry of Materials, 2010, 22, 4591-4601.	3.2	15
107	Simulation Study on the Adsorption Properties of Linear Alkanes on Closed Nanotube Bundles. Journal of Physical Chemistry B, 2012, 116, 9812-9819.	1.2	15
108	Improving the accuracy of computing chemical potentials in CFCMC simulations. Molecular Physics, 2019, 117, 3493-3508.	0.8	15

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109	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
110	Advanced Monte Carlo simulations of the adsorption of chiral alcohols in a homochiral metalâ€organic framework. AIChE Journal, 2014, 60, 2324-2334.	1.8	14
111	Aqueous Solutions of Ionic Liquids: Microscopic Assembly. ChemPhysChem, 2016, 17, 380-386.	1.0	14
112	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
113	Understanding and Exploiting Window Effects for Adsorption and Separations of Hydrocarbons. Journal of Physical Chemistry C, 2015, 119, 19236-19243.	1.5	13
114	Flexible Force Field Parameterization through Fitting on the Ab Initio-Derived Elastic Tensor. Journal of Chemical Theory and Computation, 2017, 13, 3722-3730.	2.3	13
115	Multiple linear regression and thermodynamic fluctuations are equivalent for computing thermodynamic derivatives from molecular simulation. Fluid Phase Equilibria, 2020, 523, 112785.	1.4	13
116	Predicting Multicomponent Adsorption Isotherms in Openâ€Metal Site Materials Using Force Field Calculations Based on Energy Decomposed Density Functional Theory. Chemistry - A European Journal, 2016, 22, 18045-18050.	1.7	11
117	Selective CO₂ adsorption in water-stable alkaline-earth based metalâ€“organic frameworks. Inorganic Chemistry Frontiers, 2018, 5, 541-549.	3.0	11
118	Competitive Adsorption of Xylenes at Chemical Equilibrium in Zeolites. Journal of Physical Chemistry C, 2021, 125, 4155-4174.	1.5	11
119	Investigating water and framework dynamics in pillared MOFs. Molecular Simulation, 2015, 41, 1379-1387.	0.9	10
120	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
121	Adsorption of Aromatics in MFI-Type Zeolites: Experiments and Framework Flexibility in Monte Carlo Simulations. Journal of Physical Chemistry C, 2020, 124, 21782-21797.	1.5	9
122	Multiple Free Energy Calculations from Single State Point Continuous Fractional Component Monte Carlo Simulation Using Umbrella Sampling. Journal of Chemical Theory and Computation, 2020, 16, 1757-1767.	2.3	9
123	Separation of Amyl Alcohol Isomers in ZIFâ€77. ChemPhysChem, 2015, 16, 2735-2738.	1.0	8
124	Effect of Water Content on Thermodynamic Properties of Compressed Hydrogen. Journal of Chemical & Engineering Data, 2021, 66, 2071-2087.	1.0	8
125	Electro-osmotic Drag and Thermodynamic Properties of Water in Hydrated Nafion Membranes from Molecular Dynamics. Journal of Physical Chemistry C, 2022, 126, 8121-8133.	1.5	8
126	Highlights of (bio-)chemical tools and visualization software for computational science. Current Opinion in Chemical Engineering, 2019, 23, 1-13.	3.8	7

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127	On the application of chiral amplification via adsorption. Chemical Engineering Science, 2010, 65, 6478-6485.	1.9	6
128	Diffusion Patterns in Zeolite MFI: The Cation Effect. Journal of Physical Chemistry C, 2018, 122, 29274-29284.	1.5	6
129	Molecular simulation of the vapor-liquid equilibria of xylene mixtures: Force field performance, and Wolf vs. Ewald for electrostatic interactions. Fluid Phase Equilibria, 2019, 485, 239-247.	1.4	6
130	Understanding and solving disorder in the substitution pattern of amino functionalized MIL-47(V). Dalton Transactions, 2016, 45, 4309-4315.	1.6	5
131	On the Application of Classical Molecular Simulations of Adsorption in Metalâ€“Organic Frameworks. , 2015, , 53-112.		5
132	Computational aspects of multi-species lattice-gas automata. Lecture Notes in Computer Science, 1999, , 339-349.	1.0	4
133	Reconciling the Relevant Site Model and dynamically corrected Transition State Theory. Chemical Physics Letters, 2010, 495, 77-79.	1.2	4
134	Role of additives and solvents in the synthesis of chiral isoreticular MOF-74 topologies. Dalton Transactions, 2021, 50, 12159-12167.	1.6	4
135	Dynamic structure factor in single- and two-species thermal GBL lattice gas. Computer Physics Communications, 2000, 129, 13-20.	3.0	3
136	Modifying the hydrophobic nature of MAF-6. Separation and Purification Technology, 2021, 277, 119422.	3.9	3
137	Parallel latice-Boltzmann simulation of fluid flow in centrifugal elutriation chambers. Lecture Notes in Computer Science, 1998, , 173-182.	1.0	2
138	Boltzmann approximation of transport properties in thermal lattice gases. Physical Review E, 2001, 63, 021109.	0.8	2
139	Reply to the Comment on â€œComputer Simulation of Incommensurate Diffusion in Zeolites:Â Understanding Window Effectsâ€• Journal of Physical Chemistry B, 2004, 108, 16330-16330.	1.2	2
140	The Influence of UiOâ€66 Metalâ€“Organic Framework Structural Defects on Adsorption and Separation of Hexane Isomers. Chemistry - A European Journal, 2022, , .	1.7	2
141	Coupling of thermal and mass diffusion in regular binary thermal lattice gases. Physical Review E, 2001, 64, 062102.	0.8	1
142	Regular Binary Thermal Lattice-Gases. Journal of Statistical Physics, 2002, 108, 283-315.	0.5	1
143	Using Aliphatic Alcohols to Tune Benzene Adsorption in MAFâ€6. Advanced Theory and Simulations, 2019, 2, 1900112.	1.3	1