

David Dubbeldam

List of Publications by Year in descending order

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143
papers

9,198
citations

53939

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citing authors

#	ARTICLE	IF	CITATIONS
1	The Influence of UiO-66 Metal-Organic Framework Structural Defects on Adsorption and Separation of Hexane Isomers. <i>Chemistry - A European Journal</i> , 2022, , .	1.7	2
2	Electro-osmotic Drag and Thermodynamic Properties of Water in Hydrated Nafion Membranes from Molecular Dynamics. <i>Journal of Physical Chemistry C</i> , 2022, 126, 8121-8133.	1.5	8
3	Recent advances in the continuous fractional component Monte Carlo methodology. <i>Molecular Simulation</i> , 2021, 47, 804-823.	0.9	38
4	Role of additives and solvents in the synthesis of chiral isoreticular MOF-74 topologies. <i>Dalton Transactions</i> , 2021, 50, 12159-12167.	1.6	4
5	Competitive Adsorption of Xylenes at Chemical Equilibrium in Zeolites. <i>Journal of Physical Chemistry C</i> , 2021, 125, 4155-4174.	1.5	11
6	Effect of Water Content on Thermodynamic Properties of Compressed Hydrogen. <i>Journal of Chemical & Engineering Data</i> , 2021, 66, 2071-2087.	1.0	8
7	New Features of the Open Source Monte Carlo Software Brick-CFCMC: Thermodynamic Integration and Hybrid Trial Moves. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3752-3757.	2.5	14
8	Modifying the hydrophobic nature of MAF-6. <i>Separation and Purification Technology</i> , 2021, 277, 119422.	3.9	3
9	In situ visualization of loading-dependent water effects in a stable metal-organic framework. <i>Nature Chemistry</i> , 2020, 12, 186-192.	6.6	53
10	Effects of Framework Flexibility on the Adsorption and Diffusion of Aromatics in MFI-Type Zeolites. <i>Journal of Physical Chemistry C</i> , 2020, 124, 24488-24499.	1.5	16
11	Multiple linear regression and thermodynamic fluctuations are equivalent for computing thermodynamic derivatives from molecular simulation. <i>Fluid Phase Equilibria</i> , 2020, 523, 112785.	1.4	13
12	Adsorption of Aromatics in MFI-Type Zeolites: Experiments and Framework Flexibility in Monte Carlo Simulations. <i>Journal of Physical Chemistry C</i> , 2020, 124, 21782-21797.	1.5	9
13	Synthesis of Chiral MOF-74 Frameworks by Post-Synthetic Modification by Using an Amino Acid. <i>Chemistry - A European Journal</i> , 2020, 26, 13957-13965.	1.7	35
14	Multiple Free Energy Calculations from Single State Point Continuous Fractional Component Monte Carlo Simulation Using Umbrella Sampling. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1757-1767.	2.3	9
15	Brick-CFCMC: Open Source Software for Monte Carlo Simulations of Phase and Reaction Equilibria Using the Continuous Fractional Component Method. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2678-2682.	2.5	32
16	Using Aliphatic Alcohols to Tune Benzene Adsorption in MAF-6. <i>Advanced Theory and Simulations</i> , 2019, 2, 1900112.	1.3	1
17	Improving Ammonia Production Using Zeolites. <i>Journal of Physical Chemistry C</i> , 2019, 123, 18475-18481.	1.5	16
18	Water-Ethanol and Methanol-Ethanol Separations Using in Situ Confined Polymer Chains in a Metal-Organic Framework. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 41383-41393.	4.0	29

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19	Negative Thermal Expansion Design Strategies in a Diverse Series of Metal-Organic Frameworks. <i>Advanced Functional Materials</i> , 2019, 29, 1904669.	7.8	48
20	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
21	Improving the accuracy of computing chemical potentials in CFCMC simulations. <i>Molecular Physics</i> , 2019, 117, 3493-3508.	0.8	15
22	Efficient Separation of Ethanol-Methanol and Ethanol-Water Mixtures Using ZIF-8 Supported on a Hierarchical Porous Mixed-Oxide Substrate. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 21126-21136.	4.0	26
23	Highlights of (bio-)chemical tools and visualization software for computational science. <i>Current Opinion in Chemical Engineering</i> , 2019, 23, 1-13.	3.8	7
24	Effect of truncating electrostatic interactions on predicting thermodynamic properties of water-methanol systems. <i>Molecular Simulation</i> , 2019, 45, 336-350.	0.9	17
25	Prediction of adsorption isotherms from breakthrough curves. <i>Microporous and Mesoporous Materials</i> , 2019, 277, 237-244.	2.2	36
26	Molecular simulation of the vapor-liquid equilibria of xylene mixtures: Force field performance, and Wolf vs. Ewald for electrostatic interactions. <i>Fluid Phase Equilibria</i> , 2019, 485, 239-247.	1.4	6
27	On flexible force fields for metal-organic frameworks: Recent developments and future prospects. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2018, 8, e1363.	6.2	49
28	iRASP: GPU-accelerated visualization software for materials scientists. <i>Molecular Simulation</i> , 2018, 44, 653-676.	0.9	112
29	Selective CO ₂ adsorption in water-stable alkaline-earth based metal-organic frameworks. <i>Inorganic Chemistry Frontiers</i> , 2018, 5, 541-549.	3.0	11
30	Adsorption equilibrium of nitrogen dioxide in porous materials. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4189-4199.	1.3	20
31	Absorption Refrigeration Cycles with Ammonia-Ionic Liquid Working Pairs Studied by Molecular Simulation. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 5442-5452.	1.8	39
32	Mechanical Properties in Metal-Organic Frameworks: Emerging Opportunities and Challenges for Device Functionality and Technological Applications. <i>Advanced Materials</i> , 2018, 30, e1704124.	11.1	165
33	Chemical potentials of water, methanol, carbon dioxide and hydrogen sulphide at low temperatures using continuous fractional component Gibbs ensemble Monte Carlo. <i>Molecular Simulation</i> , 2018, 44, 405-414.	0.9	17
34	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
35	Diffusion Patterns in Zeolite MFI: The Cation Effect. <i>Journal of Physical Chemistry C</i> , 2018, 122, 29274-29284.	1.5	6
36	Polarizable Force Field for CO ₂ in M-MOF-74 Derived from Quantum Mechanics. <i>Journal of Physical Chemistry C</i> , 2018, 122, 24488-24498.	1.5	29

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37	Computation of partial molar properties using continuous fractional component Monte Carlo. <i>Molecular Physics</i> , 2018, 116, 3331-3344.	0.8	28
38	Elucidating the Variable-Temperature Mechanical Properties of a Negative Thermal Expansion Metal-Organic Framework. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 21079-21083.	4.0	27
39	Polarizable Force Fields for CO ₂ and CH ₄ Adsorption in M-MOF-74. <i>Journal of Physical Chemistry C</i> , 2017, 121, 4659-4673.	1.5	87
40	Effective Model for Olefin/Paraffin Separation using (Co, Fe, Mn, Ni)-MOF-74. <i>ChemistrySelect</i> , 2017, 2, 665-672.	0.7	16
41	Behavior of the Enthalpy of Adsorption in Nanoporous Materials Close to Saturation Conditions. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3326-3339.	2.3	41
42	Computation of thermodynamic properties in the continuous fractional component Monte Carlo Gibbs ensemble. <i>Molecular Simulation</i> , 2017, 43, 189-195.	0.9	20
43	Product shape selectivity of MFI-type, MEL-type, and BEA-type zeolites in the catalytic hydroconversion of heptane. <i>Journal of Catalysis</i> , 2017, 353, 54-62.	3.1	44
44	Efficient Application of Continuous Fractional Component Monte Carlo in the Reaction Ensemble. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4452-4466.	2.3	37
45	Flexible Force Field Parameterization through Fitting on the Ab Initio-Derived Elastic Tensor. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3722-3730.	2.3	13
46	Solubility of sulfur compounds in commercial physical solvents and an ionic liquid from Monte Carlo simulations. <i>Fluid Phase Equilibria</i> , 2017, 433, 50-55.	1.4	29
47	Investigating polarization effects of CO ₂ adsorption in MgMOF-74. <i>Journal of Computational Science</i> , 2016, 15, 86-94.	1.5	25
48	Optimization of Particle Transfers in the Gibbs Ensemble for Systems with Strong and Directional Interactions Using CBMC, CFCMC, and CB/CFCMC. <i>Journal of Physical Chemistry C</i> , 2016, 120, 9148-9159.	1.5	18
49	Controlling Thermal Expansion: A Metal-Organic Frameworks Route. <i>Chemistry of Materials</i> , 2016, 28, 8296-8304.	3.2	42
50	Predicting Multicomponent Adsorption Isotherms in Open-Metal Site Materials Using Force Field Calculations Based on Energy Decomposed Density Functional Theory. <i>Chemistry - A European Journal</i> , 2016, 22, 18045-18050.	1.7	11
51	Aqueous Solutions of Ionic Liquids: Microscopic Assembly. <i>ChemPhysChem</i> , 2016, 17, 380-386.	1.0	14
52	Computation of the Heat and Entropy of Adsorption in Proximity of Inflection Points. <i>Journal of Physical Chemistry C</i> , 2016, 120, 1727-1738.	1.5	21
53	Direct Free Energy Calculation in the Continuous Fractional Component Gibbs Ensemble. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1481-1490.	2.3	47
54	Understanding and solving disorder in the substitution pattern of amino functionalized MIL-47(V). <i>Dalton Transactions</i> , 2016, 45, 4309-4315.	1.6	5

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55	Computing bubble-points of CO ₂ /CH ₄ gas mixtures in ionic liquids from Monte Carlo simulations. <i>Fluid Phase Equilibria</i> , 2016, 418, 100-107.	1.4	9
56	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
57	RASPA: molecular simulation software for adsorption and diffusion in flexible nanoporous materials. <i>Molecular Simulation</i> , 2016, 42, 81-101.	0.9	1,266
58	Separation of Amyl Alcohol Isomers in ZIF-77. <i>ChemPhysChem</i> , 2015, 16, 2735-2738.	1.0	8
59	Exploiting Large-Pore Metal-Organic Frameworks for Separations through Entropic Molecular Mechanisms. <i>ChemPhysChem</i> , 2015, 16, 2046-2067.	1.0	27
60	Entropic Separation of Styrene/Ethylbenzene Mixtures by Exploitation of Subtle Differences in Molecular Configurations in Ordered Crystalline Nanoporous Adsorbents. <i>Langmuir</i> , 2015, 31, 3771-3778.	1.6	46
61	Simulating the Reactions of CO ₂ in Aqueous Monoethanolamine Solution by Reaction Ensemble Monte Carlo Using the Continuous Fractional Component Method. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2661-2669.	2.3	30
62	Understanding DABCO Nanorotor Dynamics in Isostructural Metal-Organic Frameworks. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 812-816.	2.1	37
63	Understanding and Exploiting Window Effects for Adsorption and Separations of Hydrocarbons. <i>Journal of Physical Chemistry C</i> , 2015, 119, 19236-19243.	1.5	13
64	Understanding Nanopore Window Distortions in the Reversible Molecular Valve Zeolite RHO. <i>Chemistry of Materials</i> , 2015, 27, 5657-5667.	3.2	42
65	Solubility of Natural Gas Species in Ionic Liquids and Commercial Solvents: Experiments and Monte Carlo Simulations. <i>Journal of Chemical & Engineering Data</i> , 2015, 60, 3039-3045.	1.0	26
66	Investigating water and framework dynamics in pillared MOFs. <i>Molecular Simulation</i> , 2015, 41, 1379-1387.	0.9	10
67	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
68	On the Application of Classical Molecular Simulations of Adsorption in Metal-Organic Frameworks. , 2015, , 53-112.		5
69	Exploring new methods and materials for enantioselective separations and catalysis. <i>Molecular Simulation</i> , 2014, 40, 585-598.	0.9	21
70	Separating Xylene Isomers by Commensurate Stacking of Xylene within Channels of MAF-8. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 7774-7778.	7.2	93
71	Advanced Monte Carlo simulations of the adsorption of chiral alcohols in a homochiral metal-organic framework. <i>AIChE Journal</i> , 2014, 60, 2324-2334.	1.8	14
72	Enantioselective adsorption of ibuprofen and lysine in metal-organic frameworks. <i>Chemical Communications</i> , 2014, 50, 10849.	2.2	52

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73	A Comparison of Advanced Monte Carlo Methods for Open Systems: CFCMC vs CBMC. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 942-952.	2.3	60
74	Adsorption of hydrogen sulphide on Metal-Organic Frameworks. <i>RSC Advances</i> , 2013, 3, 14737.	1.7	49
75	On the inner workings of Monte Carlo codes. <i>Molecular Simulation</i> , 2013, 39, 1253-1292.	0.9	325
76	Strategies to Simultaneously Enhance the Hydrostability and the Alcohol-Water Separation Behavior of Cu-BTC. <i>Journal of Physical Chemistry C</i> , 2013, 117, 20706-20714.	1.5	23
77	Molecular-level Insight into Unusual Low Pressure CO ₂ Affinity in Pillared Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2013, 135, 7172-7180.	6.6	100
78	Molecular Mechanisms for Adsorption in Cu-BTC Metal Organic Framework. <i>Journal of Physical Chemistry C</i> , 2013, 117, 11357-11366.	1.5	81
79	Simulation Study of Structural Changes in Zeolite RHO. <i>Journal of Physical Chemistry C</i> , 2013, 117, 11592-11599.	1.5	23
80	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
81	Simulation Study on the Adsorption Properties of Linear Alkanes on Closed Nanotube Bundles. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9812-9819.	1.2	15
82	Feasibility of zeolitic imidazolate framework membranes for clean energy applications. <i>Energy and Environmental Science</i> , 2012, 5, 7637.	15.6	154
83	Self-Diffusion of Chain Molecules in the Metal-Organic Framework IRMOF-1: Simulation and Experiment. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 930-933.	2.1	59
84	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
85	Molecular simulation investigation into the performance of Cu-BTC metal-organic frameworks for carbon dioxide-methane separations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20453.	1.3	25
86	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
87	Elucidating steric effects on enantioselective epoxidation catalyzed by (salen)Mn in metal-organic frameworks. <i>Journal of Molecular Catalysis A</i> , 2011, 334, 89-97.	4.8	40
88	Reconciling the Relevant Site Model and dynamically corrected Transition State Theory. <i>Chemical Physics Letters</i> , 2010, 495, 77-79.	1.2	4
89	Enantioselective Adsorption in Achiral Zeolites. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 3010-3013.	7.2	36
90	On the application of chiral amplification via adsorption. <i>Chemical Engineering Science</i> , 2010, 65, 6478-6485.	1.9	6

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91	Distance and angular holonomic constraints in molecular simulations. <i>Journal of Chemical Physics</i> , 2010, 133, 034114.	1.2	16
92	Self-Diffusion Studies in CuBTC by PFG NMR and MD Simulations. <i>Journal of Physical Chemistry C</i> , 2010, 114, 10527-10534.	1.5	82
93	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
94	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
95	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
96	Effective Monte Carlo Scheme for Multicomponent Gas Adsorption and Enantioselectivity in Nanoporous Materials. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 2154-2158.	2.1	14
97	Enantioselective Adsorption Characteristics of Aluminum-Substituted MFI Zeolites. <i>Chemistry of Materials</i> , 2010, 22, 4591-4601.	3.2	15
98	Strategies for Characterization of Large-Pore Metal-Organic Frameworks by Combined Experimental and Computational Methods. <i>Chemistry of Materials</i> , 2009, 21, 4768-4777.	3.2	68
99	Method for Analyzing Structural Changes of Flexible Metal~Organic Frameworks Induced by Adsorbates. <i>Journal of Physical Chemistry C</i> , 2009, 113, 19317-19327.	1.5	71
100	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
101	Evaluation of various water models for simulation of adsorption in hydrophobic zeolites. <i>Molecular Simulation</i> , 2009, 35, 1067-1076.	0.9	60
102	Heats of Adsorption for Seven Gases in Three Metal~Organic Frameworks: Systematic Comparison of Experiment and Simulation. <i>Langmuir</i> , 2009, 25, 7383-7388.	1.6	212
103	A new perspective on the order- n algorithm for computing correlation functions. <i>Molecular Simulation</i> , 2009, 35, 1084-1097.	0.9	82
104	Transferable Force Field for Carbon Dioxide Adsorption in Zeolites. <i>Journal of Physical Chemistry C</i> , 2009, 113, 8814-8820.	1.5	199
105	Understanding Inflections and Steps in Carbon Dioxide Adsorption Isotherms in Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2008, 130, 406-407.	6.6	485
106	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
107	Separation and Molecular-Level Segregation of Complex Alkane Mixtures in Metal~Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2008, 130, 10884-10885.	6.6	116
108	Unraveling the Argon Adsorption Processes in MFI-Type Zeolite. <i>Journal of Physical Chemistry C</i> , 2008, 112, 9976-9979.	1.5	57

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109	Recent developments in the molecular modeling of diffusion in nanoporous materials. <i>Molecular Simulation</i> , 2007, 33, 305-325.	0.9	166
110	A Simulation Study of Alkanes in Linde Type A Zeolites. <i>Adsorption Science and Technology</i> , 2007, 25, 417-427.	1.5	32
111	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
112	A Computational Method To Characterize Framework Aluminum in Aluminosilicates. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 276-278.	7.2	44
113	Exceptional Negative Thermal Expansion in Isoreticular Metal-Organic Frameworks. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 4496-4499.	7.2	289
114	Molecular simulation of adsorption sites of light gases in the metal-organic framework IRMOF-1. <i>Fluid Phase Equilibria</i> , 2007, 261, 152-161.	1.4	129
115	A computational study of CO ₂ , N ₂ , and CH ₄ adsorption in zeolites. <i>Adsorption</i> , 2007, 13, 469-476.	1.4	159
116	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
117	Loading Dependence of the Diffusion Coefficient of Methane in Nanoporous Materials. <i>Journal of Physical Chemistry B</i> , 2006, 110, 22754-22772.	1.2	80
118	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
119	Understanding Diffusion in Nanoporous Materials. <i>Physical Review Letters</i> , 2006, 96, 044501.	2.9	104
120	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
121	Understanding cage effects in the n-alkane conversion on zeolites. <i>Journal of Catalysis</i> , 2006, 237, 278-290.	3.1	61
122	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
123	Molecular Understanding of Diffusion in Confinement. <i>Physical Review Letters</i> , 2005, 95, 164505.	2.9	48
124	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
125	Molecular simulation of loading-dependent diffusion in nanoporous materials using extended dynamically corrected transition state theory. <i>Journal of Chemical Physics</i> , 2005, 122, 224712.	1.2	142
126	Molecular Simulation of Loading Dependent Slow Diffusion in Confined Systems. <i>Physical Review Letters</i> , 2004, 93, 248301.	2.9	108

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127	Force Field Parametrization through Fitting on Inflection Points in Isotherms. <i>Physical Review Letters</i> , 2004, 93, 088302.	2.9	144
128	The selectivity of <i>n</i> -hexane hydroconversion on MOR-, MAZ-, and FAU-type zeolites. <i>Journal of Catalysis</i> , 2004, 228, 121-129.	3.1	28
129	Reply to the Comment on "Computer Simulation of Incommensurate Diffusion in Zeolites: A Understanding Window Effects"; <i>Journal of Physical Chemistry B</i> , 2004, 108, 16330-16330.	1.2	2
130	On the Inflection in the Concentration Dependence of the Maxwell-Stefan Diffusivity of CF ₄ in MFI Zeolite. <i>Journal of Physical Chemistry B</i> , 2004, 108, 14820-14822.	1.2	26
131	United Atom Force Field for Alkanes in Nanoporous Materials. <i>Journal of Physical Chemistry B</i> , 2004, 108, 12301-12313.	1.2	314
132	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
133	Understanding the Window Effect in Zeolite Catalysis. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 3624-3626.	7.2	68
134	Computer Simulation of Incommensurate Diffusion in Zeolites: A Understanding Window Effects. <i>Journal of Physical Chemistry B</i> , 2003, 107, 12138-12152.	1.2	83
135	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
136	Incommensurate Diffusion in Confined Systems. <i>Physical Review Letters</i> , 2003, 90, 245901.	2.9	89
137	Regular Binary Thermal Lattice-Gases. <i>Journal of Statistical Physics</i> , 2002, 108, 283-315.	0.5	1
138	Coupling of thermal and mass diffusion in regular binary thermal lattice gases. <i>Physical Review E</i> , 2001, 64, 062102.	0.8	1
139	Boltzmann approximation of transport properties in thermal lattice gases. <i>Physical Review E</i> , 2001, 63, 021109.	0.8	2
140	The distributed ASCI Supercomputer project. <i>Operating Systems Review (ACM)</i> , 2000, 34, 76-96.	1.5	80
141	Dynamic structure factor in single- and two-species thermal GBL lattice gas. <i>Computer Physics Communications</i> , 2000, 129, 13-20.	3.0	3
142	Computational aspects of multi-species lattice-gas automata. <i>Lecture Notes in Computer Science</i> , 1999, , 339-349.	1.0	4
143	Parallel lattice-Boltzmann simulation of fluid flow in centrifugal elutriation chambers. <i>Lecture Notes in Computer Science</i> , 1998, , 173-182.	1.0	2