Anne Boutin

List of Publications by Year
in descending order

145 papers	7,518 citations	47409 49 h-index	68831 81 g-index
149 all docs	149 docs citations	149 times ranked	6001 citing authors

#	Article	IF	Citations
1	Open questions on water confined in nanoporous materials. Communications Chemistry, 2021, 4, .	2.0	15
2	Structure, Dynamics, and Thermodynamics of Intruded Electrolytes in ZIF-8. Journal of Physical Chemistry C, 2019, 123, 15589-15598.	1.5	22
3	On the use of the IAST method for gas separation studies in porous materials with gate-opening behavior. Adsorption, 2018, 24, 233-241.	1.4	30
4	Structure and Dynamics of Solvated Polymers near a Silica Surface: On the Different Roles Played by Solvent. Journal of Physical Chemistry B, 2018, 122, 4573-4582.	1.2	9
5	Classical Polarizable Force Field To Study Hydrated Charged Clays and Zeolites. Journal of Physical Chemistry C, 2018, 122, 24690-24704.	1.5	16
6	Structure and Dynamics of Water Confined in Imogolite Nanotubes. Langmuir, 2018, 34, 6748-6756.	1.6	22
7	Kinetic Accessibility of Porous Material Adsorption Sites Studied through the Lattice Boltzmann Method. Langmuir, 2017, 33, 1405-1411.	1.6	14
8	Classical Polarizable Force Field To Study Dry Charged Clays and Zeolites. Journal of Physical Chemistry C, 2017, 121, 9833-9846.	1.5	11
9	Transport and adsorption under liquid flow: the role of pore geometry. Soft Matter, 2017, 13, 875-885.	1.2	31
10	New Molecular Simulation Method To Determine Both Aluminum and Cation Location in Cationic Zeolites. Chemistry of Materials, 2017, 29, 513-523.	3.2	34
11	Forced intrusion of water and aqueous solutions in microporous materials: from fundamental thermodynamics to energy storage devices. Chemical Society Reviews, 2017, 46, 7421-7437.	18.7	78
12	Cation Migration and Structural Deformations upon Dehydration of Nickel-Exchanged NaY Zeolite: A Combined Neutron Diffraction and Monte Carlo Study. Journal of Physical Chemistry C, 2016, 120, 18115-18125.	1.5	11
13	Heterometallic Metalâ€“Organic Frameworks of MOF-5 and UiO-66 Families: Insight from Computational Chemistry. Journal of Physical Chemistry C, 2016, 120, 24885-24894.	1.5	43
14	Mechanism of water adsorption in the large pore form of the gallium-based MIL-53 metal-organic framework. Microporous and Mesoporous Materials, 2016, 222, 145-152.	2.2	14
15	Novel Porous Polymorphs of Zinc Cyanide with Rich Thermal and Mechanical Behavior. Chemistry of Materials, 2015, 27, 4422-4430.	3.2	14
16	Unexpected coupling between flow and adsorption in porous media. Soft Matter, 2015, 11, 6125-6133.	1.2	27
17	Cation redistribution upon dehydration of Na₅₈Y faujasite zeolite: a joint neutron diffraction and molecular simulation study. Molecular Simulation, 2015, 41, 1371-1378.	0.9	9
18	Hydrothermal Breakdown of Flexible Metalâ€“Organic Frameworks: A Study by First-Principles Molecular Dynamics. Journal of Physical Chemistry Letters, 2015, 6, 4365-4370.	2.1	23

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19	Softening upon Adsorption in Microporous Materials: A Counterintuitive Mechanical Response. Journal of Physical Chemistry Letters, 2015, 6, 4265-4269.	2.1	20
20	Thermal and mechanical stability of zeolitic imidazolate frameworks polymorphs. APL Materials, 2014, 2, .	2.2	99
21	Molecular simulation of zeolite flexibility. Molecular Simulation, 2014, 40, 6-15.	0.9	21
22	A thermodynamic description of the adsorption-induced structural transitions in flexible MIL-53 metal-organic framework. Molecular Physics, 2014, 112, 1257-1261.	0.8	18
23	Challenges in first-principles NPT molecular dynamics of soft porous crystals: A case study on MIL-53(Ga). Journal of Chemical Physics, 2014, 141, 064703.	1.2	25
24	Remarkable Pressure Responses of Metalâ€“Organic Frameworks: Proton Transfer and Linker Coiling in Zinc Alkyl Gates. Journal of the American Chemical Society, 2014, 136, 11540-11545.	6.6	82
25	Prediction of flexibility of metalâ€“organic frameworks CAU-13 and NOTT-300 by first principles molecular simulations. Chemical Communications, 2014, 50, 5867.	2.2	46
26	Water Adsorption in Flexible Gallium-Based MIL-53 Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2014, 118, 5397-5405.	1.5	55
27	What makes zeolitic imidazolate frameworks hydrophobic or hydrophilic? The impact of geometry and functionalization on water adsorption. Physical Chemistry Chemical Physics, 2014, 16, 9940-9949.	1.3	142
28	Reorientational Dynamics of Water Confined in Zeolites. ChemPhysChem, 2014, 15, 521-529.	1.0	42
29	Metalâ€“organic frameworks with wine-rack motif: What determines their flexibility and elastic properties?. Journal of Chemical Physics, 2013, 138, 174703.	1.2	139
30	Adsorption induced transitions in soft porous crystals: An osmotic potential approach to multistability and intermediate structures. Journal of Chemical Physics, 2013, 138, 174706.	1.2	74
31	Hydrothermal and Mechanical Stability of Metal-Organic Frameworks. , 2013, , .		0
32	Adsorption Deformation and Structural Transitions in Metalâ€“Organic Frameworks: From the Unit Cell to the Crystal. Journal of Physical Chemistry Letters, 2013, 4, 3198-3205.	2.1	148
33	Investigation of structure and dynamics of the hydrated metalâ€“organic framework MIL-53(Cr) using first-principles molecular dynamics. Physical Chemistry Chemical Physics, 2013, 15, 19049.	1.3	50
34	Temperature-Induced Structural Transitions in the Gallium-Based MIL-53 Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2013, 117, 8180-8188.	1.5	59
35	Investigating the Pressure-Induced Amorphization of Zeolitic Imidazolate Framework ZIF-8: Mechanical Instability Due to Shear Mode Softening. Journal of Physical Chemistry Letters, 2013, 4, 1861-1865.	2.1	148
36	Adsorption-Induced Breathing Transitions in Metal-Organic Frameworks. , 2013, , .		0

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37	Understanding adsorption-induced structural transitions in metal-organic frameworks: From the unit cell to the crystal. Journal of Chemical Physics, 2012, 137, 184702.	1.2	35
38	Anisotropic Elastic Properties of Flexible Metal-Organic Frameworks: How Soft are Soft Porous Crystals?. Physical Review Letters, 2012, 109, 195502.	2.9	265
39	Molecular Simulation of a Znâ€“Triazamacrocyle Metalâ€“Organic Frameworks Family with Extraframework Anions. Journal of Physical Chemistry C, 2012, 116, 2952-2959.	1.5	5
40	Extension of Marcus Picture for Electron Transfer Reactions with Large Solvation Changes. Journal of the American Chemical Society, 2012, 134, 2067-2074.	6.6	42
41	Predicting Mixture Coadsorption in Soft Porous Crystals: Experimental and Theoretical Study of CO₂/CH₄ in MIL-53(Al). Langmuir, 2012, 28, 494-498.	1.6	45
42	Transferable Force Field for Carboxylate Esters: Application to Fatty Acid Methylic Ester Phase Equilibria Prediction. Journal of Physical Chemistry B, 2012, 116, 3239-3248.	1.2	27
43	Experiment and Theory of Low-Pressure Nitrogen Adsorption in Organic Layers Supported or Grafted on Inorganic Adsorbents: Toward a Tool To Characterize Surfaces of Hybrid Organic/Inorganic Systems. Langmuir, 2012, 28, 9526-9534.	1.6	15
44	Structural Changes in Nanoporous MFI Zeolites Induced by Tetrachloroethene Adsorption: A Joint Experimental and Simulation Study. Journal of Physical Chemistry C, 2011, 115, 3854-3865.	1.5	9
45	Structural Transitions in MIL-53 (Cr): View from Outside and Inside. Langmuir, 2011, 27, 4734-4741.	1.6	143
46	A Transferable Force Field To Predict Phase Equilibria and Surface Tension of Ethers and Glycol Ethers. Journal of Physical Chemistry B, 2011, 115, 10654-10664.	1.2	45
47	Mechanism of Breathing Transitions in Metalâ€“Organic Frameworks. Journal of Physical Chemistry Letters, 2011, 2, 2033-2037.	2.1	74
48	Understanding the Equilibrium Ion Exchange Properties in Faujasite Zeolite from Monte Carlo Simulations. Journal of Physical Chemistry B, 2011, 115, 15059-15066.	1.2	37
49	Thermodynamic Methods and Models to Study Flexible Metalâ€“Organic Frameworks. ChemPhysChem, 2011, 12, 247-258.	1.0	105
50	Thermodynamic analysis of the breathing of amino-functionalized MIL-53(Al) upon CO2 adsorption. Microporous and Mesoporous Materials, 2011, 140, 108-113.	2.2	78
51	Evidence of a framework induced cation redistribution upon water adsorption in cobalt exchanged X faujasite zeolite: A joint experimental and simulation study. Microporous and Mesoporous Materials, 2011, 138, 45-50.	2.2	46
52	Stress-Based Model for the Breathing of Metalâ"Organic Frameworks. Journal of Physical Chemistry Letters, 2010, 1, 445-449.	2.1	209
53	Ethanoled gasoline bubble pressure determination: Experimental and Monte Carlo modeling. Fluid Phase Equilibria, 2010, 299, 132-140.	1.4	12
54	The Behavior of Flexible MIL-53(Al) upon CH₄and CO₂Adsorption. Journal of Physical Chemistry C, 2010, 114, 22237-22244.	1.5	197

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55	Monte Carlo Simulations of Mixtures Involving Ketones and Aldehydes by a Direct Bubble Pressure Calculation. Journal of Physical Chemistry B, 2010, 114, 8680-8688.	1.2	32
56	Thermodynamic study of water confinement in hydrophobic zeolites by Monte Carlo simulations. Molecular Simulation, 2009, 35, 24-30.	0.9	27
57	Breathing Transitions in MILâ€53(Al) Metalâ€“Organic Framework Upon Xenon Adsorption. Angewandte Chemie - International Edition, 2009, 48, 8314-8317.	7.2	176
58	Transferable Force Field for Alcohols and Polyalcohols. Journal of Physical Chemistry B, 2009, 113, 5985-5995.	1.2	65
59	Unusual Hysteresis Loop in the Adsorptionâ^'Desorption of Water in NaY Zeolite at Very Low Pressure. Journal of Physical Chemistry C, 2009, 113, 8287-8295.	1.5	34
60	Double Structural Transition in Hybrid Material MIL-53 upon Hydrocarbon Adsorption: The Thermodynamics Behind the Scenes. Journal of the American Chemical Society, 2009, 131, 3442-3443.	6.6	72
61	Cation Behavior in Faujasite Zeolites upon Water Adsorption: A Combination of Monte Carlo and Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2009, 113, 10696-10705.	1.5	37
62	Hydrated Electron Diffusion: The Importance of Hydrogen-Bond Dynamics. Journal of Physical Chemistry B, 2009, 113, 11943-11949.	1.2	12
63	Prediction of Breathing and Gate-Opening Transitions Upon Binary Mixture Adsorption in Metalâ^'Organic Frameworks. Journal of the American Chemical Society, 2009, 131, 11329-11331.	6.6	144
64	Water nanodroplets confined in zeolite pores. Faraday Discussions, 2009, 141, 377-398.	1.6	71
65	A molecular simulation study of the distribution of cation inÂzeolites. Adsorption, 2008, 14, 743-754.	1.4	32
66	Does Water Condense in Hydrophobic Cavities? A Molecular Simulation Study of Hydration in Heterogeneous Nanopores. Journal of Physical Chemistry C, 2008, 112, 10435-10445.	1.5	63
67	Thermodynamics of Guest-Induced Structural Transitions in Hybrid Organicâ^'Inorganic Frameworks. Journal of the American Chemical Society, 2008, 130, 14294-14302.	6.6	299
68	Thermodynamics of water intrusion in nanoporous hydrophobic solids. Physical Chemistry Chemical Physics, 2008, 10, 4817.	1.3	103
69	Optimisation of the dynamical behaviour of the anisotropic united atom model of branched alkanes: application to the molecular simulation of fuel gasoline. Molecular Simulation, 2008, 34, 211-230.	0.9	24
70	Structural changes in nanoporous solids due to fluid adsorption: thermodynamic analysis and Monte Carlo simulations. Chemical Communications, 2008, , 3275.	2.2	38
71	Thermodynamic study of water intrusion in hydrophobic zeolites by Monte Carlo simulations. Studies in Surface Science and Catalysis, 2008, 174, 683-688.	1.5	3
72	Mechanism and kinetics of hydrated electron diffusion. Journal of Chemical Physics, 2008, 129, 054505.	1.2	10

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73	Influence of defects on the water intrusion in silicalite-1 zeolite: confrontation of experimental and molecular simulation results. Studies in Surface Science and Catalysis, 2008, 174, 561-564.	1.5	6
74	Temperature Effect on the Absorption Spectrum of the Hydrated Electron Paired with a Lithium Cation in Deuterated Water. Journal of Physical Chemistry A, 2007, 111, 3548-3553.	1.1	11
75	The Effect of Local Defects on Water Adsorption in Silicalite-1 Zeolite:â€‰ A Joint Experimental and Molecular Simulation Study. Langmuir, 2007, 23, 10131-10139.	1.6	181
76	Molecular simulation applied to fluid properties in the oil and gas industry. Molecular Simulation, 2007, 33, 287-304.	0.9	34
77	Methodology for the Calculation of the Potential of Mean Force for a Cationâ€“Ï€ Complex in Water. ChemPhysChem, 2007, 8, 1648-1656.	1.0	8
78	Adsorption of n-alkanes in faujasite zeolites: molecular simulation study and experimental measurements. Adsorption, 2007, 13, 439-451.	1.4	38
79	Molecular simulation studies of water physisorption in zeolites. Physical Chemistry Chemical Physics, 2006, 8, 5396.	1.3	139
80	Molecular Dynamics Simulations of Electronâ^'Alkali Cation Pairs in Bulk Water. Journal of Physical Chemistry B, 2006, 110, 607-615.	1.2	15
81	Adsorption of n-Alkanes in Faujasite Zeolites: Molecular Simulation Study and Experimental Measurements. Adsorption Science and Technology, 2006, 24, 713-735.	1.5	6
82	Confinement effect on the hydrated electron behaviour. Chemical Physics Letters, 2006, 428, 68-72.	1.2	7
83	Dipole Moment, Hydrogen Bonding and IR Spectrum of Confined Water. ChemPhysChem, 2006, 7, 2464-2467.	1.0	91
84	Molecular dynamics simulations of the temperature and density dependence of the absorption spectra of hydrated electron and solvated silver atom in water. Chemical Physics Letters, 2005, 409, 219-223.	1.2	14
85	Adsorption of water in zeolite sodium-faujasite. Comptes Rendus Chimie, 2005, 8, 485-490.	0.2	49
86	Adsorption of Water and Aromatics in Faujasite Zeolites: A Molecular Simulation Study. Adsorption, 2005, 11, 279-282.	1.4	14
87	Adsorption of Various Hydrocarbons in Siliceous Zeolites: A Molecular Simulation Study. Adsorption, 2005, 11, 379-382.	1.4	11
88	Water Condensation in Hydrophobic Silicalite-1 Zeolite:Â A Molecular Simulation Study. Journal of Physical Chemistry B, 2005, 109, 24071-24076.	1.2	128
89	Molecular dynamics simulations of the Ag+ or Na+ cation with an excess electron in bulk water. Journal of Chemical Physics, 2004, 120, 5261-5268.	1.2	30
90	THEORETICAL STUDY OF NEUTRAL DIPOLAR ATOM IN WATER: STRUCTURE, SPECTROSCOPY AND FORMATION OF AN EXCITONIC STATE. Modern Physics Letters B, 2004, 18, 1327-1345.	1.0	3

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91	Adsorption of Linear Alkanes in Zeolite Ferrierite from Molecular Simulations. Molecular Simulation, 2004, 30, 593-599.	0.9	8
92	Reactivity of an Excess Electron with Monovalent Cations in Bulk Water by Mixed Quantum Classical Molecular Dynamics Simulations. Molecular Simulation, 2004, 30, 749-754.	0.9	3
93	Monte Carlo versus molecular dynamics simulations in heterogeneous systems: An application to the n-pentane liquid-vapor interface. Journal of Chemical Physics, 2004, 121, 12559.	1.2	71
94	Optimized Intermolecular Potential for Aromatic Hydrocarbons Based on Anisotropic United Atoms. 1. Benzene. Journal of Physical Chemistry B, 2004, 108, 14109-14114.	1.2	50
95	A Numerical Evidence for Nonframework Cation Redistribution Upon Water Adsorption in Faujasite Zeolite. ChemPhysChem, 2004, 5, 1791-1793.	1.0	37
96	Prediction of thermodynamic derivative properties of natural condensate gases at high pressure by Monte Carlo simulation. Fluid Phase Equilibria, 2004, 220, 211-223.	1.4	56
97	Adsorption of hydrocarbons in zeolites from molecular simulations. The alkaneâ€“ferrierite system revisited. Physical Chemistry Chemical Physics, 2004, 6, 2015-2017.	1.3	14
98	Distribution of Sodium Cations in Faujasite-Type Zeolite:Â A Canonical Parallel Tempering Simulation Study. Journal of Physical Chemistry B, 2004, 108, 399-404.	1.2	79
99	Force Field Optimization for Organic Mercury Compounds. Journal of Physical Chemistry B, 2004, 108, 8419-8426.	1.2	6
100	Development of a Transferable Guestâ"Host Force Field for Adsorption of Hydrocarbons in Zeolites. II. Prediction of Alkenes Adsorption and Alkane/Alkene Selectivity in Silicalite. Journal of Physical Chemistry B, 2004, 108, 393-398.	1.2	57
101	Development of a transferable guestâ€“host force field for adsorption of hydrocarbons in zeolites : I. Reinvestigation of alkane adsorption in silicalite by grand canonical Monte Carlo simulation. Physical Chemistry Chemical Physics, 2003, 5, 3684-3693.	1.3	107
102	An optimized potential for phase equilibria calculation for ketone and aldehyde molecular fluids. Physical Chemistry Chemical Physics, 2003, 5, 4175-4179.	1.3	17
103	Molecular simulation of a hydrated electron at different thermodynamic state points. Journal of Chemical Physics, 2003, 118, 9689-9696.	1.2	66
104	Molecular Dynamics Simulations of a Silver Atom in Water: Evidence for a Dipolar Excitonic State. Physical Review Letters, 2003, 91, 208304.	2.9	28
105	New optimization method for intermolecular potentials: Optimization of a new anisotropic united atoms potential for olefins: Prediction of equilibrium properties. Journal of Chemical Physics, 2003, 118, 3020-3034.	1.2	142
106	Application of molecular simulation in the gibbs ensemble to predict liquid-vapor equilibrium curve of acetonitrile. Computer Aided Chemical Engineering, 2003, 14, 653-658.	0.3	2
107	Monte Carlo simulation of branched alkanes and long chain n -alkanes with anisotropic united atoms intermolecular potential. Molecular Simulation, 2002, 28, 317-336.	0.9	79
108	Cation distribution in faujasite-type zeolites: A test of semi-empirical force fields for Na cations. Molecular Simulation, 2002, 28, 1049-1062.	0.9	18

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109	Prediction of Equilibrium Properties of Cyclic Alkanes by Monte Carlo SimulationNew Anisotropic United Atoms Intermolecular PotentialNew Transfer Bias Method. Journal of Physical Chemistry B, 2002, 106, 5483-5491.	1.2	88
110	Direct Monte Carlo simulations of the equilibrium properties ofn-pentane liquidâ€“vapor interface. Journal of Chemical Physics, 2002, 116, 8106-8117.	1.2	75
111	Vapour-Liquid Phase Equilibria of n-alkanes by Direct Monte Carlo Simulations. Molecular Simulation, 2001, 27, 99-114.	0.9	41
112	Molecular Simulation of Adsorption of Guest Molecules in Zeolitic Materials: A Comparative Study of Intermolecular Potentials. Molecular Simulation, 2001, 27, 371-385.	0.9	8
113	Placement of cations in NaX faujasite-type zeolite using (N,V,T) Monte Carlo simulations. Chemical Communications, 2001, , 2200-2201.	2.2	25
114	Direct calculation of bubble points for alkane mixtures by molecular simulation. Molecular Physics, 2001, 99, 1423-1434.	0.8	20
115	Molecular simulation of adsorption equilibria of xylene isomer mixtures in faujasite zeolites. A study of the cation exchange effect on adsorption selectivity. Physical Chemistry Chemical Physics, 2001, 3, 80-86.	1.3	35
116	A Simple Model for Predicting the Na+Distribution in Anhydrous NaY and NaX Zeolites. Journal of Physical Chemistry B, 2001, 105, 9569-9575.	1.2	120
117	Monte Carlo Simulations of Ag+ and Ag in Aqueous Solution. Redox Potential of the Ag+/Ag Couple. Journal of Physical Chemistry B, 2001, 105, 9363-9369.	1.2	22
118	Prediction of thermodynamic derivative properties of fluids by Monte Carlo simulation. Physical Chemistry Chemical Physics, 2001, 3, 4333-4339.	1.3	110
119	Optimization of the anisotropic united atoms intermolecular potential forn-alkanes. Journal of Chemical Physics, 2000, 112, 5499-5510.	1.2	270
120	Molecular Simulation of Vapour-Liquid Coexistence Curves for Hydrogen Sulfide-Alkane and Carbon Dioxide-Alkane Mixtures. Molecular Simulation, 1999, 22, 351-368.	0.9	28
121	Vapour-liquid coexistence curves of the united-atom and anisotropic united-atom force fields for alkane mixtures. Molecular Physics, 1999, 96, 1517-1524.	0.8	34
122	Direct calculation of bubble points by Monte Carlo simulation. Molecular Physics, 1999, 97, 523-539.	0.8	30
123	From molecular clusters to bulk matter. II. Crossover from icosahedral to crystalline structures in CO2 clusters. Journal of Chemical Physics, 1999, 111, 2095-2102.	1.2	32
124	Molecular simulations on volumetric properties of natural gas. Fluid Phase Equilibria, 1999, 161, 45-62.	1.4	18
125	Monte Carlo simulations of squalane in the Gibbs ensemble. Fluid Phase Equilibria, 1999, 155, 167-176.	1.4	16
126	Molecular Simulation of p-Xylene and m-Xylene Adsorption in Y Zeolites. Single Components and Binary Mixtures Study. Langmuir, 1999, 15, 8678-8685.	1.6	62

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127	Computational Study ofp-Xylene/m-Xylene Mixtures Adsorbed in NaY Zeolite. Journal of Physical Chemistry B, 1998, 102, 9224-9233.	1.2	75
128	From molecular clusters to bulk matter. I. Structure and thermodynamics of small CO2, N2, and SF6 clusters. Journal of Chemical Physics, 1998, 109, 329-337.	1.2	64
129	The Melting Phase Transition in Small Carbon Dioxide Clusters. Molecular Simulation, 1997, 19, 285-299.	0.9	6
130	Grand canonical Monte Carlo simulations of adsorption of mixtures of xylene molecules in faujasite zeolites. Faraday Discussions, 1997, 106, 307-323.	1.6	68
131	Vapour-Liquid Phase Equilibria Predictions of Methaneâ€“Alkane Mixtures by Monte Carlo Simulation. Molecular Simulation, 1997, 19, 1-15.	0.9	79
132	Intermolecular Potential Functions for Adsorption in Zeolites: State of the Art and Effective Models. Molecular Simulation, 1996, 17, 217-238.	0.9	20
133	The Adsorption of Argon and Nitrogen in Silicalite-1 Zeolite: A Grand Canonical Monte-Carlo study. Molecular Simulation, 1996, 17, 255-288.	0.9	30
134	Numerical Evidence of an Embryonic Orientational Phase Transition in Small Nitrogen Clusters. Physical Review Letters, 1996, 76, 4336-4339.	2.9	28
135	Molecular Simulation Study of the Structural Rearrangement of Methane Adsorbed in Aluminophosphate AlPO4-5. The Journal of Physical Chemistry, 1996, 100, 9006-9013.	2.9	75
136	Objections to the Hotspot Model for the unidentified infrared emission bands of the interstellar medium. Monthly Notices of the Royal Astronomical Society, 1995, 274, 435-438.	1.6	2
137	The temperature-size phase diagram of large SF6 clusters by computer simulation. Chemical Physics Letters, 1994, 218, 122-127.	1.2	26
138	Molecular simulation of the stepped adsorption isotherm of methane in AlPO4-5. Chemical Physics Letters, 1994, 219, 484-490.	1.2	46
139	The phase transitions of sulphur hexafluoride by molecular dynamics simulation. Molecular Physics, 1994, 81, 1165-1176.	0.8	4
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145	Is There a Vacancy-Induced Premelting in a Molecular Crystal?. Europhysics Letters, 1992, 18, 245-250.	0.7	16