Peter A Monson

List of Publications by Year
in descending order

149 papers	7,247 citations	47006 47 h-index	62596 80 g-index
159 all docs	159 docs citations	159 times ranked	4228 citing authors

#	Article	IF	Citations
1	Tailored Porous Materials. Chemistry of Materials, 1999, 11, 2633-2656.	6.7	714
2	Adsorption in Porous Materials at High Pressure:Â Theory and Experiment. Langmuir, 2002, 18, 10261-10273.	3.5	344
3	Capillary Condensation in Disordered Porous Materials: Hysteresis versus Equilibrium Behavior. Physical Review Letters, 2001, 87, 055701.	7.8	261
4	Modeling of Adsorption and Desorption in Pores of Simple Geometry Using Molecular Dynamics. Langmuir, 2001, 17, 7600-7604.	3.5	247
5	Exploration of molecular dynamics during transient sorption of fluids in mesoporous materials. Nature, 2006, 443, 965-968.	27.8	218
6	Monte Carlo calculations of cluster statistics in continuum models of composite morphology. Journal of Chemical Physics, 1988, 88, 1198-1206.	3.0	179
7	Physical adsorption of gases: the case for absolute adsorption as the basis for thermodynamic analysis. Adsorption, 2014, 20, 591-622.	3.0	137
8	Prewetting at a fluid-solid interface via Monte Carlo simulation. Physical Review A, 1989, 39, 6402-6408.	2.5	134
9	Solidâ€“fluid equilibria for hard dumbbells via Monte Carlo simulation. Journal of Chemical Physics, 1992, 96, 9060-9072.	3.0	130
10	Substitutionally ordered solid solutions of hard spheres. Journal of Chemical Physics, 1995, 102, 3354-3360.	3.0	127
11	Phase behavior and dynamics of fluids in mesoporous glasses. Physical Review E, 2003, 67, 041207.	2.1	121
12	Monte Carlo Simulation Studies of Heats of Adsorption in Heterogeneous Solids. Langmuir, 1996, 12, 5425-5432.	3.5	111
13	Does Water Condense in Carbon Pores?. Langmuir, 2005, 21, 10219-10225.	3.5	107
14	Phase diagrams of single-component fluids in disordered porous materials: Predictions from integral-equation theory. Journal of Chemical Physics, 1997, 106, 264-279.	3.0	106
15	Adsorption/Desorption Hysteresis in Inkbottle Pores:Â A Density Functional Theory and Monte Carlo Simulation Study. Langmuir, 2004, 20, 4289-4294.	3.5	100
16	Adsorption of fluids in disordered porous media from integral equation theory. Journal of Chemical Physics, 1993, 99, 3003-3013.	3.0	98
17	Phase equilibrium in a molecular model of a fluid confined in a disordered porous material. Physical Review E, 1996, 54, R29-R32.	2.1	98
18	The influence of adsorbent microstructure upon adsorption equilibria: Investigations of a model system. Journal of Chemical Physics, 1991, 95, 2936-2948.	3.0	91

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19	Density Functional Theory Study of Silica Zeolite Structures:Â Stabilities and Mechanical Properties of SOD, LTA, CHA, MOR, and MFI. Journal of Physical Chemistry B, 2004, 108, 9208-9215.	2.6	89
20	Monte Carlo calculations of phase diagrams for a fluid confined in a disordered porous material. Physical Review E, 1996, 54, 6557-6564.	2.1	87
21	Crystal nucleation in binary hard sphere mixtures: A Monte Carlo simulation study. Journal of Chemical Physics, 2006, 125, 024508.	3.0	86
22	Adsorption hysteresis and capillary condensation in disordered porous solids: a density functional study. Journal of Physics Condensed Matter, 2002, 14, 9295-9315.	1.8	85
23	Hysteresis in Monte Carlo and Molecular Dynamics Simulations of Adsorption in Porous Materials. Langmuir, 2000, 16, 9857-9860.	3.5	83
24	Mean-Field Theory of Fluid Adsorption in a Porous Glass. Langmuir, 2001, 17, 7472-7475.	3.5	83
25	Lattice model of adsorption in disordered porous materials: Mean-field density functional theory and Monte Carlo simulations. Physical Review E, 2001, 65, 011202.	2.1	80
26	Understanding capillary condensation and hysteresis in porous silicon: Network effects within independent pores. Physical Review E, 2008, 78, 060601.	2.1	80
27	Mean field kinetic theory for a lattice gas model of fluids confined in porous materials. Journal of Chemical Physics, 2008, 128, 084701.	3.0	80
28	Modeling Spontaneous Formation of Precursor Nanoparticles in Clear-Solution Zeolite Synthesis. Journal of the American Chemical Society, 2005, 127, 14388-14400.	13.7	79
29	On the stability of the plastic crystal phase of hard dumbbell solids. Journal of Chemical Physics, 1992, 97, 8543-8548.	3.0	76
30	Modeling Mercury Porosimetry Using Statistical Mechanics. Langmuir, 2004, 20, 6482-6489.	3.5	76
31	Monte Carlo Simulation Study of Water Adsorption in Activated Carbon. Industrial & Engineering Chemistry Research, 2006, 45, 5649-5656.	3.7	73
32	Solid-Fluid Equilibrium: Insights from Simple Molecular Models. Advances in Chemical Physics, 2007, , 113-179.	0.3	73
33	Solidâ€“fluid equilibrium for a molecular model with short ranged directional forces. Journal of Chemical Physics, 1998, 109, 9938-9949.	3.0	68
34	Contact Angles, Pore Condensation, and Hysteresis: Insights from a Simple Molecular Model. Langmuir, 2008, 24, 12295-12302.	3.5	67
35	Understanding adsorption and desorption processes in mesoporous materials with independent disordered channels. Physical Review E, 2009, 80, 031607.	2.1	67
36	Calculation of Free Energies and Chemical Potentials for Gas Hydrates Using Monte Carlo Simulations. Journal of Physical Chemistry B, 2007, 111, 7274-7282.	2.6	66

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37	Computer simulations of phase equilibrium for a fluid confined in a disordered porous structure. Physical Review E, 2000, 61, 7231-7234.	2.1	59
38	Mean-Field Theory of Liquid Droplets on Roughened Solid Surfaces:Â Application to Superhydrophobicity. Langmuir, 2006, 22, 1595-1601.	3.5	59
39	The high density equation of state and solid-fluid equilibrium in systems of freely jointed chains of tangent hard spheres. Journal of Chemical Physics, 1997, 107, 6899-6907.	3.0	58
40	Plastic crystal phases of hard dumbbells and hard spherocylinders. Journal of Chemical Physics, 1997, 107, 2696-2697.	3.0	58
41	Mercury Porosimetry in Mesoporous Glasses:Â A Comparison of Experiments with Results from a Molecular Model. Langmuir, 2007, 23, 3372-3380.	3.5	57
42	Probing Memory Effects in Confined Fluids via Diffusion Measurements. Langmuir, 2008, 24, 6429-6432.	3.5	56
43	Recent Progress in the Statistical Mechanical Mechanics of Interaction Site Fluids. Advances in Chemical Physics, 2007, , 451-550.	0.3	55
44	Modeling Desorption of Fluids from Disordered Mesoporous Materials. Langmuir, 2004, 20, 4743-4747.	3.5	52
45	Vapour-liquid equilibria for two centre Lennard-Jones diatomics and dipolar diatomics. Molecular Physics, 1993, 80, 997-1007.	1.7	50
46	Solid-fluid equilibrium in molecular models of n-alkanes. Journal of Chemical Physics, 1999, 110, 664-675.	3.0	50
47	Solution of the Ornsteinâ€“Zernike equation in the vicinity of the critical point of a simple fluid. Journal of Chemical Physics, 1985, 82, 4303-4311.	3.0	49
48	Further studies of prewetting transitions via Monte Carlo simulation. Journal of Chemical Physics, 1993, 99, 6897-6906.	3.0	49
49	A cell theory for solid solutions: Application to hard sphere mixtures. Journal of Chemical Physics, 1993, 99, 8914-8921.	3.0	45
50	Molecular Modeling of Adsorption in Activated Carbon: Comparison of Monte Carlo Simulations with Experiment. Adsorption, 2005, 11, 5-13.	3.0	44
51	Theory of monolayer physical adsorption. II. Fluid phases on a periodic surface. Journal of Chemical Physics, 1981, 74, 6431-6439.	3.0	43
52	Numerical solution of the RISM equations for the site-site 12-6 potential. Molecular Physics, 1982, 47, 435-442.	1.7	42
53	Liquidâ€“liquid equilibrium in a slit pore: Monte Carlo simulation and mean field density functional theory. Journal of Chemical Physics, 1995, 102, 3712-3719.	3.0	42
54	On the mechanical properties and phase behavior of silica: A simple model based on low coordination and strong association. Journal of Chemical Physics, 2004, 121, 8415.	3.0	41

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55	Probing the Mechanism of Silica Polymerization at Ambient Temperatures using Monte Carlo Simulations. Journal of Physical Chemistry Letters, 2010, 1, 3219-3224.	4.6	41
56	Virial equation of state for rigid spherocylinders. Molecular Physics, 1978, 35, 1337-1342.	1.7	40
57	Monte Carlo Simulations of Silica Polymerization and Network Formation. Journal of Physical Chemistry C, 2011, 115, 15988-16000.	3.1	40
58	Dynamic Aspects of Mercury Porosimetry:Â A Lattice Model Study. Langmuir, 2005, 21, 3179-3186.	3.5	35
59	Solidâ€“fluid equilibria for quadrupolar hard dumbbells via Monte Carlo simulation. Journal of Chemical Physics, 1995, 102, 1361-1372.	3.0	34
60	Modeling Relaxation Processes for Fluids in Porous Materials Using Dynamic Mean Field Theory: AnÂApplication to Partial Wetting. Journal of Low Temperature Physics, 2009, 157, 395-409.	1.4	34
61	Mixtures of hard spherocylinders and hard spheres. Molecular Physics, 1980, 39, 977-988.	1.7	33
62	Cluster perturbation theory for interaction site fluids. Journal of Chemical Physics, 1987, 87, 3618-3629.	3.0	33
63	Multiscale Model for the Templated Synthesis of Mesoporous Silica: The Essential Role of Silica Oligomers. Chemistry of Materials, 2016, 28, 2715-2727.	6.7	32
64	Modeling the Impact of Mesoporous Silica Microstructures on the Adsorption Hysteresis Loop. Journal of Physical Chemistry C, 2020, 124, 21646-21655.	3.1	32
65	Calculating the Phase Behavior of Gas-Hydrate-Forming Systems from Molecular Models. Industrial & Engineering Chemistry Research, 2006, 45, 424-431.	3.7	31
66	Molecular Simulations of the Synthesis of Periodic Mesoporous Silica Phases at High Surfactant Concentrations. Journal of Physical Chemistry C, 2017, 121, 4564-4575.	3.1	29
67	Molecular Modeling of Mercury Porosimetry. Adsorption, 2005, 11, 325-329.	3.0	28
68	Filling Dynamics of Closed End Nanocapillaries. Langmuir, 2014, 30, 1290-1294.	3.5	28
69	Modelling the assembly of nanoporous silica materials. International Reviews in Physical Chemistry, 2015, 34, 35-70.	2.3	28
70	Phase behavior of a hard sphere interaction site model of benzene. Journal of Chemical Physics, 2000, 112, 8950-8957.	3.0	27
71	Thermodynamic properties of molecular fluids from the site-site Ornstein-Zernike equation. Molecular Physics, 1984, 53, 1209-1223.	1.7	26
72	Solidâ€fluid equilibrium in a nonlinear hard sphere triatomic model of propane. Journal of Chemical Physics, 1995, 103, 9756-9762.	3.0	26

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73	Equilibrium properties of the Gaussian overlap fluid. Monte Carlo simulation and thermodynamic perturbation theory. The Journal of Physical Chemistry, 1983, 87, 2852-2858.	2.9	25
74	Modeling the Influence of Heterogeneous Adsorbent Microstructure upon Adsorption Equilibria for Binary Mixtures. Langmuir, 1994, 10, 530-537.	3.5	25
75	A molecular model of adsorption in a dilute semiflexible porous network. Molecular Physics, 2002, 100, 2031-2039.	1.7	25
76	Monte Carlo simulation study of adsorption from a liquid mixture at states near liquidâ€“liquid coexistence. Journal of Chemical Physics, 1993, 99, 8238-8243.	3.0	24
77	Integral equations for polar molecular fluids. Molecular Physics, 1983, 48, 181-191.	1.7	23
78	Solidâ€“fluid phase equilibrium for single component and binary Lennardâ€Jones systems: A cell theory approach. Journal of Chemical Physics, 1996, 105, 10022-10029.	3.0	23
79	Dynamic mean field theory of condensation and evaporation processes for fluids in porous materials: Application to partial drying and drying. Faraday Discussions, 2010, 146, 167.	3.2	23
80	Molecular dynamics simulations of hard sphere solidification at constant pressure. Physical Review E, 2001, 64, 061703.	2.1	22
81	Phase equilibrium in a quadrupolar hard sphere interaction site model of benzene. Journal of Chemical Physics, 2001, 114, 4124-4130.	3.0	22
82	Modeling Nanoparticle Formation during Early Stages of Zeolite Growth: A Low-Coordination Lattice Model of Template Penetration. Journal of Physical Chemistry C, 2010, 114, 14393-14401.	3.1	22
83	Simulating the Formation of Surfactant-Templated Mesoporous Silica Materials: A Model with Both Surfactant Self-Assembly and Silica Polymerization. Langmuir, 2013, 29, 766-780.	3.5	22
84	Recent Progress in Molecular Modeling of Adsorption and Hysteresis in Mesoporous Materials. Adsorption, 2005, 11, 29-35.	3.0	21
85	Normal mode approach for predicting the mechanical properties of solids from first principles: Application to compressibility and thermal expansion of zeolites. Physical Review B, 2005, 71, .	3.2	21
86	Wetting of rings on a nanopatterned surface: A lattice model study. Physical Review E, 2006, 73, 041603.	2.1	21
87	Computer simulation of adsorption equilibrium for a gas on a solid surface using the potential distribution theory. Journal of Chemical Physics, 1986, 84, 1909-1915.	3.0	20
88	Reply to â€˜â€˜Comment on â€˜Prewetting at a solid-fluid interface via Monte Carlo simulationâ€™ â€™â€™. Physical Review A, 1990, 42, 2458-2459.	2.5	20
89	Modelling the thermal stability of precursor nanoparticles in zeolite synthesis. Molecular Physics, 2006, 104, 3513-3522.	1.7	20
90	Dynamics of capillary condensation in lattice gas models of confined fluids: A comparison of dynamic mean field theory with dynamic Monte Carlo simulations. Journal of Chemical Physics, 2013, 138, 234709.	3.0	20

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91	Prewetting at a liquid mixtureâ€“solid interface: A comparison of Monte Carlo simulations with mean field density functional theory. Journal of Chemical Physics, 1994, 101, 10947-10952.	3.0	19
92	Understanding congruent melting in binary solids: Molecular models of benzeneâ€“hexafluorobenzene mixtures. Journal of Chemical Physics, 2003, 118, 2815.	3.0	19
93	Modeling three-dimensional network formation with an atomic lattice model: Application to silicic acid polymerization. Journal of Chemical Physics, 2011, 134, 134703.	3.0	19
94	Solidâ€“fluid and solidâ€“solid phase equilibrium in a model of n-alkane mixtures. Journal of Chemical Physics, 2004, 120, 2980-2988.	3.0	18
95	Physical adsorption in heterogeneous porous materials: an analytical study of a one-dimensional model. Langmuir, 1993, 9, 561-567.	3.5	17
96	Diffusion hysteresis in mesoporous materials. European Physical Journal: Special Topics, 2007, 141, 107-112.	2.6	17
97	Modeling the Self-Assembly of Silica-Templated Nanoparticles in the Initial Stages of Zeolite Formation. Langmuir, 2015, 31, 4940-4949.	3.5	17
98	Clustering and percolation in assemblies of anisotropic particles: Perturbation theory and Monte Carlo simulation. Physical Review A, 1988, 38, 5376-5383.	2.5	16
99	Phase diagrams of a fluid confined in a disordered porous material. Journal of Physics Condensed Matter, 1996, 8, 9621-9625.	1.8	16
100	Morphology of Fluids Confined in Physically Reconstructed Mesoporous Silica: Experiment and Mean Field Density Functional Theory. Langmuir, 2018, 34, 9936-9945.	3.5	16
101	Non-additive three body contributions to the lattice energies of nitrogen and carbon dioxide. Molecular Physics, 1980, 39, 1163-1168.	1.7	15
102	An interaction site approach to clustering and percolation phenomena in systems of nonspherical particles. Journal of Chemical Physics, 1988, 89, 3300-3307.	3.0	15
103	An analysis of the statistical model adsorption isotherm. AICHE Journal, 1992, 38, 1979-1989.	3.6	15
104	Surface Roughness Effects in Molecular Models of Adsorption in Heterogeneous Porous Solids. Langmuir, 1998, 14, 4880-4886.	3.5	15
105	Solidâ^'Fluid and Solidâ^'Solid Equilibrium in Hard Sphere United Atom Models of n-Alkanes: Rotator Phase Stability. Journal of Physical Chemistry B, 2009, 113, 13866-13873.	2.6	15
106	On the pair distribution function in fluids of hard non-spherical molecules. Molecular Physics, 1979, 38, 1699-1702.	1.7	14
107	Equilibrium properties of molecular fluids with charge distributions of quadrupolar symmetry. Journal of Chemical Physics, 1983, 78, 4126-4132.	3.0	14
108	Deviations from two-dimensionality in classical adsorbed films. Surface Science, 1982, 122, 401-407.	1.9	13

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109	Cluster integrals for square well particles: Application to percolation. Journal of Chemical Physics, 1991, 94, 3070-3082.	3.0	13
110	A study of the phase behavior of a simple model of chiral molecules and enantiomeric mixtures. Journal of Chemical Physics, 2005, 122, 054505.	3.0	13
111	Further studies of a simple atomistic model of silica: Thermodynamic stability of zeolite frameworks as silica polymorphs. Journal of Chemical Physics, 2007, 126, 144701.	3.0	13
112	Studies of a Lattice Model of Water Confined in a Slit Pore. Journal of Physical Chemistry C, 2007, 111, 15976-15981.	3.1	13
113	Molecular thermodynamics of solidâ€fluid and solidâ€solid equilibria. AICHE Journal, 2008, 54, 1122-1128.	3.6	13
114	Emergence of Zeolite Analogs and other Microporous Crystals in an Atomic Lattice Model of Silica and Related Materials. Journal of Physical Chemistry Letters, 2012, 3, 761-765.	4.6	13
115	Sorption Isotherm Reconstruction and Extraction of Pore Size Distributions for Serially Connected Pore Model (SCPM) Structures Employing Algorithmic and Statistical Models. Journal of Physical Chemistry C, 2020, 124, 21591-21607.	3.1	13
116	An application of classical thermodynamics to solid-fluid equilibrium in hard sphere mixtures. Journal of Chemical Physics, 1997, 107, 6855-6858.	3.0	12
117	The phase behavior of a hard sphere chain model of a binaryn-alkane mixture. Journal of Chemical Physics, 2000, 112, 2870-2877.	3.0	12
118	Dynamical aspects of the adsorption hysteresis phenomenon. Magnetic Resonance Imaging, 2007, 25, 481-484.	1.8	11
119	Dynamic density functional theory with hydrodynamic interactions: Theoretical development and application in the study of phase separation in gas-liquid systems. Journal of Chemical Physics, 2015, 142, 094706.	3.0	11
120	Lattice Model for Silica Polymerization: Monte Carlo Simulations of the Transition between Gel and Nanoparticle Phases. Journal of Physical Chemistry B, 2014, 118, 10989-10999.	2.6	10
121	Reactive Ensemble Monte Carlo Simulations of Silica Polymerization That Yield Zeolites and Related Crystalline Microporous Structures. Journal of Physical Chemistry C, 2015, 119, 26628-26635.	3.1	10
122	Solution of the Percus-Yevick equation in the coexistence region of a simple fluid. International Journal of Thermophysics, 1985, 6, 573-584.	2.1	9
123	Local compositions and the square-well fluid. International Journal of Thermophysics, 1986, 7, 367-379.	2.1	9
124	Isobaric ensemble Monte Carlo simulation of adsorption at fluid-solid interfaces. Langmuir, 1989, 5, 639-644.	3.5	9
125	Dynamic Mean Field Theory for Lattice Gas Models of Fluid Mixtures Confined in Mesoporous Materials. Langmuir, 2013, 29, 13808-13820.	3.5	9
126	Lattice Monte Carlo Simulations in Search of Zeolite Analogues: Effects of Structure Directing Agents. Journal of Physical Chemistry C, 2015, 119, 28046-28054.	3.1	9

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127	An application of cell theory to molecular models of n-alkane solids. Molecular Physics, 2000, 98, 363-370.	1.7	8
128	Dynamic mean field theory for lattice gas models of fluids confined in porous materials: Higher order theory based on the Bethe-Peierls and path probability method approximations. Journal of Chemical Physics, 2014, 141, 024706.	3.0	8
129	Modeling fluids confined in three-dimensionally ordered mesoporous carbons. Adsorption, 2021, 27, 253-264.	3.0	8
130	On series expansions of orientation-dependent properties of pairs of non-spherical molecules. Molecular Physics, 1983, 49, 251-274.	1.7	7
131	Isobaric molecular dynamics simulations of hard sphere systems. Physical Review E, 2001, 63, 061106.	2.1	7
132	Modelling relaxation processes for fluids in porous materials using dynamic mean field theory: application to pore networks. Adsorption, 2011, 17, 769-776.	3.0	7
133	Modeling the Role of Excluded Volume in Zeolite Structure Direction. Journal of Physical Chemistry Letters, 2018, 9, 3703-3707.	4.6	7
134	Nonequilibrium Steady States in Fluid Transport through Mesopores: Dynamic Mean Field Theory and Nonequilibrium Molecular Dynamics. Langmuir, 2019, 35, 5702-5710.	3.5	7
135	A new method for the numerical solution of integral equation approximations. International Journal of Thermophysics, 1990, 11, 97-107.	2.1	6
136	Mean-field theory of ice phase stability. Journal of Chemical Physics, 2003, 118, 7005-7011.	3.0	6
137	Modelling the dynamics of condensation and evaporation of fluids in three-dimensional slit pores. Molecular Physics, 2015, 113, 1250-1260.	1.7	6
138	On the mechanical stability of the body-centered cubic phase and the emergence of a metastable cI16 phase in classical hard sphere solids. Journal of Chemical Physics, 2018, 148, 024502.	3.0	6
139	Modeling permporometry of mesoporous membranes using dynamic mean field theory. AICHE Journal, 2015, 61, 2958-2967.	3.6	5
140	Additions and corrections. Equilibrium Properties of the Gaussian Overlap Fluid. The Journal of Physical Chemistry, 1984, 88, 2678-2678.	2.9	4
141	Modeling the Influence of Side Stream and Ink Bottle Structures on Adsorption/Desorption Dynamics of Fluids in Long Pores. Langmuir, 2015, 31, 188-198.	3.5	4
142	Enhanced replica exchange reactive Monte Carlo simulations for constructing zeolite frameworks. Molecular Simulation, 2018, 44, 453-462.	2.0	4
143	Modeling Mesoscale Structure in Comb Polymer Materials for Anhydrous Proton Transport Applications. Macromolecules, 2010, 43, 9549-9554.	4.8	3
144	Studies of a primitive model of mixtures of nonpolar molecules with water. Molecular Physics, 2004, 102, 2071-2079.	1.7	2

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145	Density-functional theory study of the body-centered-cubic and cI16 hard-sphere crystals. Journal of Chemical Physics, 2019, 150, 134506.	3.0	2
146	Connecting dynamic pore filling mechanisms with equilibrium and out of equilibrium configurations of fluids in nanopores. Journal of Chemical Physics, 2022, 156, 134702.	3.0	2
147	A comparison of dynamic mean field theory and grand canonical molecular dynamics for the dynamics of pore filling and capillary condensation of fluids in mesopores. Journal of Chemical Physics, 2018, 149, 014703.	3.0	1
148	Heats of Adsorption from Molecular Models of Adsorption in Heterogeneous Solids. Kluwer International Series in Engineering and Computer Science, 1996, , 1009-1018.	0.2	1
149	Comment on â€œComputer Simulation of Static and Dynamic Properties During Transient Sorption of Fluids in Mesoporous Materialsâ€. Journal of Physical Chemistry C, 2010, 114, 9187-9188.	3.1	0