List of Publications by Year in descending order

338 papers	30,106 citations	6233 80 h-index	6282 158 g-index
344 all docs	344 docs citations	344 times ranked	13025 citing authors

#	Article	IF	Citations
1	Current Advances in Characterization of Nano-porous Materials: Pore Size Distribution and Surface Area. Engineering Materials, 2021, , 315-340.	0.3	10
2	Can we define a unique microscopic pressure in inhomogeneous fluids?. Journal of Chemical Physics, 2021, 154, 084502.	1.2	12
3	Gerhard Findenegg (1938â€“2019). Molecular Physics, 2021, 119, .	0.8	0
4	Enhancing Gas Solubility in Nanopores: A Combined Study Using Classical Density Functional Theory and Machine Learning. Langmuir, 2020, 36, 8527-8536.	1.6	20
5	The Youngâ€“Laplace equation for a solidâ€“liquid interface. Journal of Chemical Physics, 2020, 153, 191102.	1.2	35
6	Microscopic Pressure Tensor in Cylindrical Geometry: Pressure of Water in a Carbon Nanotube. Journal of Chemical Theory and Computation, 2020, 16, 5548-5561.	2.3	14
7	Conformal Sites Theory for Adsorbed Films on Energetically Heterogeneous Surfaces. Langmuir, 2020, 36, 1822-1838.	1.6	7
8	Reply to the â€˜Comment on â€œPressure enhancement in carbon nanopores: a major confinement effectâ€â€™ by D. van Dijk, Phys. Chem. Chem. Phys., 2020, 22, DOI: 10.1039/C9CP02890K. Physical Chemistry Chemical Physics, 2020, 22, 9826-9830.	1.3	9
9	Structure of ice confined in carbon and silica nanopores. Bulletin of Materials Science, 2019, 42, 1.	0.8	4
10	Bottom-Up Approach to the Coarse-Grained Surface Model: Effective Solidâ€“Fluid Potentials for Adsorption on Heterogeneous Surfaces. Langmuir, 2019, 35, 5975-5986.	1.6	17
11	The Nitric Oxide Dimer Reaction in Carbon Nanopores. Journal of Physical Chemistry B, 2018, 122, 3604-3614.	1.2	17
12	Effect of Confinement on Melting in Nanopores. , 2018, , .		1
13	The pressure in interfaces having cylindrical geometry. Journal of Chemical Physics, 2018, 149, 084109.	1.2	9
14	Surface-Driven High-Pressure Processing. Engineering, 2018, 4, 311-320.	3.2	11
15	High-density equation of state for a two-dimensional Lennard-Jones solid. Journal of Chemical Physics, 2018, 148, 174505.	1.2	9
16	Computer simulation of conductive linear sulfur chains confined in carbon nanotubes. Molecular Simulation, 2017, 43, 519-525.	0.9	14
17	Molecular Modeling and Adsorption Properties of Ordered Silica-Templated CMK Mesoporous Carbons. Langmuir, 2017, 33, 2109-2121.	1.6	15
18	Adhesion and friction in polymer films on solid substrates: conformal sites analysis and corresponding surface measurements. Soft Matter, 2017, 13, 3492-3505.	1.2	16

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19	Pressure Enhancement in Confined Fluids: Effect of Molecular Shape and Fluidâ€“Wall Interactions. Langmuir, 2017, 33, 11231-11245.	1.6	30
20	Computationally Mapping pK_a Shifts Due to the Presence of a Polyelectrolyte Chain around Whey Proteins. Langmuir, 2017, 33, 11417-11428.	1.6	32
21	Effect of confinement in nano-porous materials on the solubility of a supercritical gas. Molecular Physics, 2016, 114, 3294-3306.	0.8	29
22	Structure of Ice in Confinement: Water in Mesoporous Carbons. Journal of Chemical & Engineering Data, 2016, 61, 4252-4260.	1.0	24
23	Liquidâ€“Solid Nanofriction and Interfacial Wetting. Langmuir, 2016, 32, 743-750.	1.6	31
24	Perturbation theories of the thermodynamics of polar and associating liquids: A historical perspective. Fluid Phase Equilibria, 2016, 416, 3-17.	1.4	41
25	Melting of Eutectic Mixtures in Silica and Carbon Nanopores. Journal of Chemical & Engineering Data, 2015, 60, 3093-3100.	1.0	2
26	Water on Titanium Dioxide Surface: A Revisiting by Reactive Molecular Dynamics Simulations. Langmuir, 2014, 30, 14832-14840.	1.6	64
27	Thermodynamics of confined nano-phases. Journal of Chemical Thermodynamics, 2014, 74, 169-183.	1.0	107
28	The theory of non-electrolyte solutions: an historical review. Molecular Physics, 2013, 111, 3666-3697.	0.8	22
29	High pressure effect in nanoporous carbon materials: Effects of pore geometry. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2013, 437, 33-41.	2.3	46
30	Controllable atomistic graphene oxide model and its application in hydrogen sulfide removal. Journal of Chemical Physics, 2013, 139, 194707.	1.2	23
31	Reactive adsorption of ammonia and ammonia/water on CuBTC metal-organic framework: A ReaxFF molecular dynamics simulation. Journal of Chemical Physics, 2013, 138, 034102.	1.2	38
32	On the molecular origin of high-pressure effects in nanoconfinement: The role of surface chemistry and roughness. Journal of Chemical Physics, 2013, 139, 144701.	1.2	57
33	Dynamics of nanoconfined water under pressure. Physical Review E, 2013, 88, 022316.	0.8	7
34	Activation of water on the TiO2 (110) surface: The case of Ti adatoms. Journal of Chemical Physics, 2012, 136, 064703.	1.2	12
35	Analysis of the solvation structure of rubidium bromide under nanoconfinement. Molecular Simulation, 2012, 38, 1209-1220.	0.9	3
36	Molecular behavior of water in TiO2 nano-slits with varying coverages of carbon: a molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2012, 14, 16536.	1.3	34

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37	Structural analysis of water and carbon tetrachloride adsorbed in activated carbon fibres. Physical Chemistry Chemical Physics, 2012, 14, 7145.	1.3	32
38	ReaxFF molecular dynamics simulation of thermal stability of a Cu3(BTC)2 metalâ€“organic framework. Physical Chemistry Chemical Physics, 2012, 14, 11327.	1.3	48
39	Under pressure: Quasi-high pressure effects in nanopores. Microporous and Mesoporous Materials, 2012, 154, 19-23.	2.2	49
40	Atomistic models for disordered nanoporous carbons using reactive force fields. Microporous and Mesoporous Materials, 2012, 154, 24-37.	2.2	76
41	Novel ice structures in carbon nanopores: pressure enhancement effect of confinement. Physical Chemistry Chemical Physics, 2011, 13, 9008.	1.3	26
42	Adsorptive behavior of CO2, CH4 and their mixtures in carbon nanospace: a molecular simulation study. Physical Chemistry Chemical Physics, 2011, 13, 3985.	1.3	66
43	Simulating Local Adsorption Isotherms in Structurally Complex Porous Materials: A Direct Assessment of the Slit Pore Model. Journal of Physical Chemistry Letters, 2011, 2, 165-169.	2.1	30
44	Pressure enhancement in carbon nanopores: a major confinement effect. Physical Chemistry Chemical Physics, 2011, 13, 17163-17170.	1.3	124
45	Toward Understanding Reactive Adsorption of Ammonia on Cu-MOF/Graphite Oxide Nanocomposites. Langmuir, 2011, 27, 13043-13051.	1.6	137
46	Adsorption, structure and dynamics of benzene in ordered and disordered porous carbons. Physical Chemistry Chemical Physics, 2011, 13, 3748-3757.	1.3	55
47	The role of molecular modeling in confined systems: impact and prospects. Physical Chemistry Chemical Physics, 2011, 13, 58-85.	1.3	153
48	Adsorption and diffusion of argon in disordered nanoporous carbons. Adsorption, 2011, 17, 189-199.	1.4	25
49	Adsorption and diffusion of argon confined in ordered and disordered microporous carbons. Applied Surface Science, 2010, 256, 5131-5136.	3.1	47
50	Ti-decorated C60 as catalyst for hydrogen generation and storage. Applied Physics Letters, 2010, 96, .	1.5	18
51	Freezing of mixtures confined in silica nanopores: Experiment and molecular simulation. Journal of Chemical Physics, 2010, 133, 084701.	1.2	28
52	Transition from single-file to Fickian diffusion for binary mixtures in single-walled carbon nanotubes. Journal of Chemical Physics, 2010, 133, 094501.	1.2	35
53	Dissociation of water over Ti-decorated C60. Journal of Chemical Physics, 2010, 133, 084510.	1.2	13
54	Molecular Modeling of Matter: Impact and Prospects in Engineering. Industrial & Engineering Chemistry Research, 2010, 49, 3026-3046.	1.8	98

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55	Melting Behavior of Bromobenzene within Carbon Nanotubesâ€. Journal of Chemical & Engineering Data, 2010, 55, 4183-4189.	1.0	15
56	Dual diffusion mechanism of argon confined in single-walled carbon nanotube bundles. Physical Chemistry Chemical Physics, 2010, 12, 6632.	1.3	25
57	Melting of mixtures in silica nanopores. Pure and Applied Chemistry, 2009, 81, 1953-1959.	0.9	25
58	Modeling Micelle-Templated Mesoporous Material SBA-15: Atomistic Model and Gas Adsorption Studies. Langmuir, 2009, 25, 5802-5813.	1.6	44
59	Adsorption and Structure of Benzene on Silica Surfaces and in Nanopores. Langmuir, 2009, 25, 10648-10659.	1.6	69
60	Energetics investigation on encapsulation of protein/peptide drugs in carbon nanotubes. Journal of Chemical Physics, 2009, 131, 015101.	1.2	35
61	Hydrogen storage enhanced in Li-doped carbon replica of zeolites: A possible route to achieve fuel cell demand. Journal of Chemical Physics, 2009, 130, 174717.	1.2	31
62	Molecular design of photoactive acenes for organic photovoltaics. Journal of Chemical Physics, 2009, 130, 194701.	1.2	19
63	Effect of Pressure on the Freezing of Pure Fluids and Mixtures Confined in Nanopores. Journal of Physical Chemistry B, 2009, 113, 13874-13881.	1.2	52
64	Isomerization kinetics of small hydrocarbons in confinement. Adsorption, 2008, 14, 181-188.	1.4	5
65	Molecular-level simulations of chemical reaction equilibrium for nitric oxide dimerization reaction in disordered nanoporous carbons. Fluid Phase Equilibria, 2008, 272, 18-31.	1.4	14
66	Simulation of chemical reaction equilibria by the reaction ensemble Monte Carlo method: a reviewâ€. Molecular Simulation, 2008, 34, 119-146.	0.9	102
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69	Molecular simulation study of temperature effect on ionic hydration in carbon nanotubes. Physical Chemistry Chemical Physics, 2008, 10, 1896.	1.3	76
70	Catalytic role of carbons in methane decomposition for CO- and CO2-free hydrogen generation. Journal of Chemical Physics, 2008, 128, 214702.	1.2	34
71	Melting behavior of water in cylindrical pores: carbon nanotubes and silica glasses. Physical Chemistry Chemical Physics, 2008, 10, 4909.	1.3	52
72	A remarkable shape-catalytic effect of confinement on the rotational isomerization of small hydrocarbons. Journal of Chemical Physics, 2008, 128, 034704.	1.2	25

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73	A Monte Carlo study of capillary condensation of krypton within realistic models of templated mesoporous silica materials. Studies in Surface Science and Catalysis, 2007, , 153-160.	1.5	8
74	Coarse Graining of Nonbonded Degrees of Freedom. Physical Review Letters, 2007, 98, 267801.	2.9	24
75	Freezing of argon in ordered and disordered porous carbon. Physical Review B, 2007, 76, .	1.1	46
76	Confinement effects on freezing of binary mixtures. Studies in Surface Science and Catalysis, 2007, 160, 667-674.	1.5	0
77	Modeling Triblock Surfactant Templated Mesoporous Silicas (MCF and SBA-15): A Mimetic Simulation Study. Studies in Surface Science and Catalysis, 2007, , 527-534.	1.5	4
78	Crossover from Normal to Inverse Temperature Dependence in the Adsorption of Nonionic Surfactants at Hydrophilic Surfaces and Pore Wallsâ€. Journal of Physical Chemistry C, 2007, 111, 16045-16054.	1.5	24
79	Molecular Dynamics Study on Diameter Effect in Structure of Ethanol Molecules Confined in Single-Walled Carbon Nanotubesâ€. Journal of Physical Chemistry C, 2007, 111, 15677-15685.	1.5	48
80	Anisotropic Self-Diffusion in Nanofluidic Structures. Journal of Physical Chemistry C, 2007, 111, 15493-15504.	1.5	13
81	Ring Connectivity:Â Measuring Network Connectivity in Network Covalent Solids. Langmuir, 2007, 23, 1123-1130.	1.6	8
82	Adsorption and dynamics of argon in porous carbons. European Physical Journal: Special Topics, 2007, 141, 121-125.	1.2	6
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84	Molecular simulation of the adsorption and structure of benzene confined in mesoporous silicas. Adsorption, 2007, 13, 485-490.	1.4	24
85	Confinement effects on chemical reactionsâ€"Toward an integrated rational catalyst design. Applied Surface Science, 2007, 253, 5570-5579.	3.1	40
86	STRUCTURAL MODELING OF POROUS CARBONS USING A HYBRID REVERSE MONTE CARLO METHOD. , 2007, , .		1
87	Molecular Modeling of Porous Carbons Using the Hybrid Reverse Monte Carlo Method. Langmuir, 2006, 22, 9942-9948.	1.6	161
88	Fast Method for Computing Pore Size Distributions of Model Materials. Langmuir, 2006, 22, 7726-7731.	1.6	242
89	Hybrid Reverse Monte Carlo Reconstruction and Simulation Studies. , 2006, , .		0
90	Adsorption of Simple Gases in MCM-41 Materials:Â The Role of Surface Roughness. Langmuir, 2006, 22, 194-202.	1.6	129

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91	Simulated water adsorption in chemically heterogeneous carbon nanotubes. Journal of Chemical Physics, 2006, 124, 074710.	1.2	76
92	Adsorption, structure and dynamics of fluids in ordered and disordered models of porous carbons. Molecular Physics, 2006, 104, 3491-3499.	0.8	37
93	Structure of saccharose-based carbon and transport of confined fluids: hybrid reverse Monte Carlo reconstruction and simulation studies. Molecular Simulation, 2006, 32, 567-577.	0.9	47
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99	Freezing of Fluids Confined in a Disordered Nanoporous Structure. Physical Review Letters, 2006, 97, 105702.	2.9	32
100	Adsorption and structure of argon in activated porous carbons. Molecular Simulation, 2006, 32, 557-566.	0.9	16
101	Adsorption and catalysis: The effect of confinement on chemical reactions. Applied Surface Science, 2005, 252, 766-777.	3.1	85
102	Temperature Effect on Adsorption/Desorption Isotherms for a Simple Fluid Confined within Various Nanopores. Adsorption, 2005, 11, 289-294.	1.4	59
103	The Effect of Pore Connectivity on Water Adsorption Isotherms in Non-Activated Graphitic Nanopores. Adsorption, 2005, 11, 337-341.	1.4	17
104	Effect of Confinement on Chemical Reactions. Adsorption, 2005, 11, 349-354.	1.4	28
105	Effects of Activation on the Structure and Adsorption Properties of a Nanoporous Carbon Using Molecular Simulation. Adsorption, 2005, 11, 355-360.	1.4	52
106	Effect of Confinement on Freezing of CCl4 in Cylindrical Pores. Adsorption, 2005, 11, 391-396.	1.4	17
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112	Cosurfactant and cosolvent effects on surfactant self-assembly in supercritical carbon dioxide. Journal of Chemical Physics, 2005, 122, 094710.	1.2	54
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117	An experimental study of melting of CCl4 in carbon nanotubes. Physical Chemistry Chemical Physics, 2005, 7, 3884.	1.3	8
118	Vaporâ˜'Liquid and Vaporâ˜'Liquidâ˜'Liquid Equilibria of Carbon Dioxide/n-Perfluoroalkane/n-Alkane Ternary Mixtures. Journal of Physical Chemistry B, 2005, 109, 2899-2910.	1.2	24
119	Effect of Temperature on the Adsorption of Water in Porous Carbons. Langmuir, 2005, 21, 9457-9467.	1.6	87
120	Water in carbon nanotubes: Adsorption isotherms and thermodynamic properties from molecular simulation. Journal of Chemical Physics, 2005, 122, 234712.	1.2	225
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125	Freezing and melting of binary mixtures confined in a nanopore. Molecular Physics, 2004, 102, 2149-2163.	0.8	30
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128	Lattice Monte Carlo Simulations of Phase Separation and Micellization in Supercritical CO2/Surfactant Systems:â€‰ Effect of CO2 Density. Langmuir, 2004, 20, 514-523.	1.6	26
129	Anomalous Temperature Dependence of Surfactant Self-Assembly from Aqueous Solution. Physical Review Letters, 2004, 92, 135701.	2.9	41
130	Molecular dynamics simulations of simple fluids confined in realistic models of nanoporous carbons. European Physical Journal E, 2003, 12, 35-40.	0.7	21
131	Pore Size Distribution of Porous Glasses:Â A Test of the Independent Pore Model. Langmuir, 2003, 19, 8592-8604.	1.6	32
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140	Influence of synthesis conditions on surface heterogeneity of M41 type materials studied with lattice Monte Carlo. Studies in Surface Science and Catalysis, 2002, 144, 647-654.	1.5	9
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144	Predictions of the Jouleâ˜'Thomson Inversion Curve for then-Alkane Series and Carbon Dioxide from the Soft-SAFT Equation of Stateâ€. Industrial & Engineering Chemistry Research, 2002, 41, 1069-1075.	1.8	39

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146	Self-assembly of surfactants in a supercritical solvent from lattice Monte Carlo simulations. Journal of Chemical Physics, 2002, 116, 1171-1184.	1.2	63
147	Simulation of chemical reaction equilibria and kinetics in heterogeneous carbon micropores. Applied Surface Science, 2002, 196, 366-374.	3.1	33
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149	Phase behavior of PVACâ€“PTAN block copolymer in supercritical carbon dioxide using SAFT. Fluid Phase Equilibria, 2002, 194-197, 553-565.	1.4	12
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151	Dielectric studies of freezing behavior in porous materials: Water and methanol in activated carbon fibres. Physical Chemistry Chemical Physics, 2001, 3, 1179-1184.	1.3	72
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173	Pore Size Distributions in Porous Glasses:Â A Computer Simulation Study. Langmuir, 1999, 15, 305-308.	1.6	438
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