J Karl Johnson

List of Publications by Year
in descending order

Version: 2024-02-01

189	14,691	14644	19726
papers	citations	66 h-index	117 g-index

197	197	197	11601
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Identifying UiOâ€67 Metalâ€Organic Framework Defects and Binding Sites through Ammonia Adsorption. ChemSusChem, 2022, 15, .	3.6	6
2	Study of self-interaction-errors in barrier heights using locally scaled and Perdewâ€“Zunger self-interaction methods. Journal of Chemical Physics, 2022, 156, 014306.	1.2	12
3	Effect of Chain Length on the Dipole Moment of Polyisobutylene Succinate Anhydride. Industrial & Engineering Chemistry Research, 2022, 61, 2359-2365.	1.8	3
4	Fermiâ€“LÃ¶wdin orbital self-interaction correction of adsorption energies on transition metal ions. Journal of Chemical Physics, 2022, 156, 134102.	1.2	2
5	Combined Deep Learning and Classical Potential Approach for Modeling Diffusion in UiO-66. Journal of Chemical Theory and Computation, 2022, 18, 3593-3606.	2.3	19
6	In Situ Nuclear Magnetic Resonance Investigation of Molecular Adsorption and Kinetics in Metalâ€“Organic Framework UiO-66. Journal of Physical Chemistry Letters, 2021, 12, 892-899.	2.1	10
7	Adsorption separation of heavier isotope gases in subnanometer carbon pores. Nature Communications, 2021, 12, 546.	5.8	18
8	Impact of defects on the decomposition of chemical warfare agent simulants in Zrâ€based metal organic frameworks. AICHE Journal, 2021, 67, e17156.	1.8	5
9	Theoretical Study of the Impact of Vacancies and Disorder on the Electronic Properties of Cu_{2â€“x}Se. Journal of Physical Chemistry C, 2021, 125, 12324-12332.	1.5	3
10	Binding of CO and O on Low-Symmetry Pt Clusters Supported on Amorphous Silica. Journal of Physical Chemistry C, 2021, 125, 13780-13787.	1.5	4
11	Efficiently Trained Deep Learning Potential for Graphane. Journal of Physical Chemistry C, 2021, 125, 14874-14882.	1.5	18
12	H₂/CO₂ separations in multicomponent metal-adeninate MOFs with multiple chemically distinct pore environments. Chemical Science, 2020, 11, 12807-12815.	3.7	18
13	Understanding and Improving the Kinetics of Bulk Carbonation on Sodium Carbonate. Journal of Physical Chemistry C, 2020, 124, 23106-23115.	1.5	5
14	Application of Self-Interaction Corrected Density Functional Theory to Early, Middle, and Late Transition States. Journal of Physical Chemistry A, 2020, 124, 8223-8234.	1.1	12
15	Modeling of Diffusion of Acetone in UiO-66. Journal of Physical Chemistry C, 2020, 124, 28469-28478.	1.5	23
16	Design, Synthesis, and Characterization of Metalâ€“Organic Frameworks for Enhanced Sorption of Chemical Warfare Agent Simulants. Journal of Physical Chemistry C, 2019, 123, 19748-19758.	1.5	33
17	Designing Open Metal Sites in Metalâ€“Organic Frameworks for Paraffin/Olefin Separations. Journal of the American Chemical Society, 2019, 141, 13003-13007.	6.6	93
18	Fundamental Insights into the Reactivity and Utilization of Open Metal Sites in Cu(I)-MFU-4l. Organometallics, 2019, 38, 3453-3459.	1.1	12

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19	Method for Predicting Dipole Moments of Complex Molecules for Use in Thermophysical Property Estimation. Industrial & Engineering Chemistry Research, 2019, 58, 19263-19270.	1.8	4
20	Test of the Duh-Haymet-Henderson theory for mixtures: cavity correlation functions and excess volumes. Molecular Physics, 2019, 117, 3623-3631.	0.8	1
21	Toward Understanding the Kinetics of CO₂ Capture on Sodium Carbonate. ACS Applied Materials & Interfaces, 2019, 11, 9033-9041.	4.0	21
22	Graphamine: Amine-Functionalized Graphane for Intrinsic Anhydrous Proton Conduction. Journal of Physical Chemistry C, 2019, 123, 1566-1571.	1.5	9
23	Energy Efficient Formaldehyde Synthesis by Direct Hydrogenation of Carbon Monoxide in Functionalized Metalâ€“Organic Frameworks. ACS Sustainable Chemistry and Engineering, 2019, 7, 2508-2515.	3.2	18
24	Unraveling Anhydrous Proton Conduction in Hydroxygraphane. Journal of Physical Chemistry Letters, 2019, 10, 518-523.	2.1	13
25	Quantum chemistry benchmarking of binding and selectivity for lanthanide extractants. International Journal of Quantum Chemistry, 2018, 118, e25516.	1.0	17
26	Shrinking Self-Interaction Errors with the Fermiâ€“LÃ¶wdin Orbital Self-Interaction-Corrected Density Functional Approximation. Journal of Physical Chemistry A, 2018, 122, 9307-9315.	1.1	30
27	TiH₂ as a Dynamic Additive for Improving the De/Rehydrogenation Properties of MgH₂: A Combined Experimental and Theoretical Mechanistic Investigation. Journal of Physical Chemistry C, 2018, 122, 21248-21261.	1.5	44
28	Mechanism of Isobutylene Polymerization: Quantum Chemical Insight into AlCl₃/H₂O-Catalyzed Reactions. ACS Catalysis, 2018, 8, 8006-8013.	5.5	19
29	The effect of topology in Lewis pair functionalized metal organic frameworks on CO₂ adsorption and hydrogenation. Catalysis Science and Technology, 2018, 8, 4609-4617.	2.1	14
30	Screening the activity of Lewis pairs for hydrogenation of CO₂. Molecular Simulation, 2017, 43, 821-827.	0.9	12
31	A comparison of the correlation functions of the Lennardâ€“Jones fluid for the first-order Duhâ€“Haymetâ€“Henderson closure with molecular simulations. Molecular Physics, 2017, 115, 1335-1342.	0.8	5
32	Adsorption and Diffusion of Fluids in Defective Carbon Nanotubes: Insights from Molecular Simulations. Langmuir, 2017, 33, 11834-11844.	1.6	9
33	Beyond Ordered Materials: Understanding Catalytic Sites on Amorphous Solids. ACS Catalysis, 2017, 7, 7543-7557.	5.5	134
34	Facile Anhydrous Proton Transport on Hydroxyl Functionalized Graphane. Physical Review Letters, 2017, 118, 186101.	2.9	21
35	Impact of Support Interactions for Single-Atom Molybdenum Catalysts on Amorphous Silica. Industrial & Engineering Chemistry Research, 2016, 55, 12350-12357.	1.8	24
36	Predicting catalyst-support interactions between metal nanoparticles and amorphous silica supports. Surface Science, 2016, 652, 278-285.	0.8	17

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37	Catalytic hydrogenation of CO₂ to methanol in a Lewis pair functionalized MOF. Catalysis Science and Technology, 2016, 6, 8392-8405.	2.1	75
38	Cavity correlation and bridge functions at high density and near the critical point: a test of second-order Percusâ€“Yevick theory. Molecular Physics, 2016, 114, 2516-2522.	0.8	7
39	Structural and Electronic Properties of Pt₁₃ Nanoclusters on Amorphous Silica Supports. Journal of Physical Chemistry C, 2015, 119, 2503-2512.	1.5	34
40	Design of Lewis Pair-Functionalized Metal Organic Frameworks for CO₂ Hydrogenation. ACS Catalysis, 2015, 5, 2921-2928.	5.5	137
41	Screening Lewis Pair Moieties for Catalytic Hydrogenation of CO₂ in Functionalized UiO-66. ACS Catalysis, 2015, 5, 6219-6229.	5.5	80
42	Effect of Support Preparation and Nanoparticle Size on Catalystâ€“Support Interactions between Pt and Amorphous Silica. Journal of Physical Chemistry C, 2015, 119, 19934-19940.	1.5	52
43	A first-principles study of lithium-decorated hybrid boron nitride and graphene domains for hydrogen storage. Journal of Chemical Physics, 2014, 141, 084711.	1.2	29
44	Accurate Amorphous Silica Surface Models from First-Principles Thermodynamics of Surface Dehydroxylation. Langmuir, 2014, 30, 5133-5141.	1.6	89
45	Utilizing the Gate-Opening Mechanism in ZIF-7 for Adsorption Discrimination between N₂O and CO₂. Journal of Physical Chemistry C, 2014, 118, 17831-17837.	1.5	51
46	Development of a ReaxFF Reactive Force Field for Tetrabutylphosphonium Glycinate/CO₂ Mixtures. Journal of Physical Chemistry B, 2014, 118, 12008-12016.	1.2	46
47	Elucidation of Aqueous Solvent-Mediated Hydrogen-Transfer Reactions by ab Initio Molecular Dynamics and Nudged Elastic-Band Studies of NaBH₄ Hydrolysis. Journal of Physical Chemistry C, 2014, 118, 21385-21399.	1.5	37
48	A Combined Experimental and Computational Study on Selected Physical Properties of Aminosilicones. Industrial & Engineering Chemistry Research, 2014, 53, 1334-1341.	1.8	7
49	Deliquescence of NaBH4 from Density Functional Theory and Experiments. Industrial & Engineering Chemistry Research, 2013, 52, 13849-13861.	1.8	4
50	Effect of Spinâ€Crossoverâ€Induced Pore Contraction on CO₂â€“Host Interactions in the Porous Coordination Polymers [Fe(pyrazine)M(CN)₄] (M = Ni, Pt). European Journal of Inorganic Chemistry, 2013, 2013, 511-519.	1.0	15
51	Gas sorption properties of zwitterion-functionalized carbon nanotubes. Journal of Membrane Science, 2013, 429, 88-94.	4.1	20
52	Systematic modulation and enhancement of CO2â€‰:â€‰N2 selectivity and water stability in an isoreticular series of bio-MOF-11 analogues. Chemical Science, 2013, 4, 1746.	3.7	182
53	Is there a Difference in Van Der Waals Interactions between Rare Gas Atoms Adsorbed on Metallic and Semiconducting Single-Walled Carbon Nanotubes?. Physical Review Letters, 2013, 110, 135503.	2.9	19
54	Experimental and Theoretical Comparison of Gas Desorption Energies on Metallic and Semiconducting Single-Walled Carbon Nanotubes. Journal of the American Chemical Society, 2013, 135, 7768-7776.	6.6	20

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55	Zwitterion Functionalized Carbon Nanotube/Polyamide Nanocomposite Membranes for Water Desalination. ACS Nano, 2013, 7, 5308-5319.	7.3	331
56	Properties of Weakly Bound Molecular Oxygen on the Rutile TiO₂(110) Surface from Density Functional Theory. Journal of Physical Chemistry C, 2013, 117, 17151-17158.	1.5	2
57	Porous Carbon Nanotube Membranes for Separation of H₂/CH₄ and CO₂/CH₄ Mixtures. Journal of Physical Chemistry C, 2012, 116, 25904-25910.	1.5	59
58	Density functional theory studies on the electronic, structural, phonon dynamical and thermo-stability properties of bicarbonates MHCO₃, M = Li, Na, K. Journal of Physics Condensed Matter, 2012, 24, 325501.	0.7	11
59	Methyl Radical Reactivity on the Basal Plane of Graphite. Journal of Physical Chemistry C, 2012, 116, 18347-18357.	1.5	16
60	Density functional theory study of CO2 capture with transition metal oxides and hydroxides. Journal of Chemical Physics, 2012, 136, 064516.	1.2	26
61	The role of van der Waals interactions in the adsorption of noble gases on metal surfaces. Journal of Physics Condensed Matter, 2012, 24, 424211.	0.7	42
62	Reaction of the Basal Plane of Graphite with the Methyl Radical. Journal of Physical Chemistry Letters, 2012, 3, 1680-1683.	2.1	21
63	Examining the robustness of first-principles calculations for metal hydride reaction thermodynamics by detection of metastable reaction pathways. Physical Chemistry Chemical Physics, 2011, 13, 21520.	1.3	14
64	A Computational Study of the Heats of Reaction of Substituted Monoethanolamine with CO₂. Journal of Physical Chemistry A, 2011, 115, 342-350.	1.1	40
65	Critical Assessment of CO₂ Solubility in Volatile Solvents at 298.15 K. Journal of Chemical & Engineering Data, 2011, 56, 1565-1572.	1.0	49
66	Molecular Simulations and Theoretical Predictions for Adsorption and Diffusion of CH₄/H₂ and CO₂/CH₄ Mixtures in ZIFs. Journal of Physical Chemistry C, 2011, 115, 12560-12566.	1.5	101
67	Methyl Chloride Reactions on Lithiated Carbon Nanotubes: Lithium as Both Reactant and Catalyst. Journal of Physical Chemistry C, 2011, 115, 11694-11700.	1.5	8
68	Large-scale screening of metal hydrides for hydrogen storage from first-principles calculations based on equilibrium reaction thermodynamics. Physical Chemistry Chemical Physics, 2011, 13, 7218.	1.3	30
69	Vacancy clusters as entry ports for cesium intercalation in graphite. Carbon, 2011, 49, 3937-3952.	5.4	28
70	CO2 capture properties of Mâ€“Câ€“Oâ€“H (M=Li, Na, K) systems: A combined density functional theory and lattice phonon dynamics study. Journal of Solid State Chemistry, 2011, 184, 304-311.	1.4	74
71	Surface reactions of AsH3, H2Se, and H2S on the Zn2TiO4(010) surface. Surface Science, 2011, 605, 818-823.	0.8	10
72	Noble gases on metal surfaces: Insights on adsorption site preference. Physical Review B, 2011, 84, .	1.1	33

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73	One-dimensional adsorption and diffusion in Zn(tbip). Molecular Simulation, 2011, 37, 640-646.	0.9	5
74	Aminosilicone Solvents for CO₂ Capture. ChemSusChem, 2010, 3, 919-930.	3.6	57
75	First principles study of vacancy and tungsten diffusion in fcc cobalt. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 015008.	0.8	13
76	Development of a Transferable Reactive Force Field for Cobalt. Journal of Physical Chemistry A, 2010, 114, 5855-5861.	1.1	41
77	First-Principles Characterization of Amorphous Phases of MB₁₂H₁₂, M = Mg, Ca. Journal of Physical Chemistry C, 2010, 114, 14601-14605.	1.5	29
78	Defect and Nondefect Interstitial Channel Availability in Carbon Nanotube Bundles: Comparison of Modeling with Experiments. Journal of Physical Chemistry C, 2010, 114, 7602-7610.	1.5	16
79	Hydrogen Isotope Separation in Carbon Nanotubes: Calculation of Coupled Rotational and Translational States at High Densities. ACS Nano, 2010, 4, 1703-1715.	7.3	46
80	Reaction Mechanism of Monoethanolamine with CO₂ in Aqueous Solution from Molecular Modeling. Journal of Physical Chemistry A, 2010, 114, 11844-11852.	1.1	161
81	Carbonâ^'Chlorine Bond Scission in Li-Doped Single-Walled Carbon Nanotubes: Reaction of CH₃Cl and Lithium. Journal of Physical Chemistry C, 2010, 114, 17148-17158.	1.5	9
82	Atomic Charges Derived from Electrostatic Potentials for Molecular and Periodic Systems. Journal of Physical Chemistry A, 2010, 114, 10225-10233.	1.1	70
83	Vibron hopping and bond anharmonicity in hot dense hydrogen. Journal of Chemical Physics, 2009, 130, 054502.	1.2	5
84	Assessing nanoparticle size effects on metal hydride thermodynamics using the Wulff construction. Nanotechnology, 2009, 20, 204001.	1.3	127
85	Solubility of CO2 in CO2-philic oligomers; COSMOtherm predictions and experimental results. Fluid Phase Equilibria, 2009, 287, 26-32.	1.4	55
86	Prediction of CH4/H2 Mixture Selectivity in Zn(tbip) from Computer Simulations. Journal of Low Temperature Physics, 2009, 157, 268-276.	0.6	20
87	Tests of Pore-Size Distributions Deduced fromÂInversion of Simulated and Real Adsorption Data. Journal of Low Temperature Physics, 2009, 157, 410-428.	0.6	24
88	Atomically detailed models of gas mixture diffusion through CuBTC membranes. Microporous and Mesoporous Materials, 2009, 125, 101-106.	2.2	90
89	Influence of tert-amine groups on the solubility of polymers in CO2. Polymer, 2009, 50, 2436-2444.	1.8	42
90	Enhancement of Adsorption Inside Single-Walled Carbon Nanotubes: Li Doping Effect on n-Heptane van der Waals Bonding. Journal of Physical Chemistry C, 2009, 113, 4829-4838.	1.5	13

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91	Adsorption and Diffusion of Light Gases in ZIF-68 and ZIF-70: A Simulation Study. Journal of Physical Chemistry C, 2009, 113, 16906-16914.	1.5	126
92	Ozone Oxidation of Single Walled Carbon Nanotubes from Density Functional Theory. Journal of Physical Chemistry C, 2009, 113, 17636-17642.	1.5	45
93	The importance of chargeâ€“quadrupole interactions for H2adsorption and diffusion in CuBTC. Molecular Simulation, 2009, 35, 60-69.	0.9	39
94	Progress, Opportunities, and Challenges for Applying Atomically Detailed Modeling to Molecular Adsorption and Transport in Metalâ^'Organic Framework Materials. Industrial & Engineering Chemistry Research, 2009, 48, 2355-2371.	1.8	283
95	Design and Evaluation of Nonfluorous CO₂-Soluble Oligomers and Polymers. Journal of Physical Chemistry B, 2009, 113, 14971-14980.	1.2	69
96	DFT characterization of adsorption and diffusion mechanisms of H, As, S, and Se on the zinc orthotitanate(010) surface. Surface Science, 2008, 602, 1877-1882.	0.8	2
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109	A corresponding states principle for physisorption and deviations for quantum fluids. Molecular Physics, 2008, 106, 1579-1585.	0.8	14
110	Reactive Canonical Monte Carlo. Advances in Chemical Physics, 2007, , 461-481.	0.3	16
111	Phase Behavior of Oxygen-Containing Polymers in CO2. Macromolecules, 2007, 40, 1332-1341.	2.2	95
112	First principles screening of destabilized metal hydrides for high capacity H2 storage using scandium. Journal of Alloys and Compounds, 2007, 446-447, 23-27.	2.8	33
113	Stability analysis of doped materials for reversible hydrogen storage in destabilized metal hydrides. Physical Review B, 2007, 76, .	1.1	26
114	First-Principles Investigation of Adsorption and Dissociation of Hydrogen on Mg2Si Surfaces. Journal of Physical Chemistry C, 2007, 111, 6910-6916.	1.5	21
115	Predicting Reaction Equilibria for Destabilized Metal Hydride Decomposition Reactions for Reversible Hydrogen Storage. Journal of Physical Chemistry C, 2007, 111, 1584-1591.	1.5	84
116	Inter- and Intratube Self-Diffusion in n-Heptane Adsorbed on Carbon Nanotubes. Journal of Physical Chemistry C, 2007, 111, 4578-4584.	1.5	16
117	Thermal Conductivity of Methane Hydrate from Experiment and Molecular Simulation. Journal of Physical Chemistry B, 2007, 111, 13194-13205.	1.2	119
118	Experimental and Theoretical Studies of Gas Adsorption in Cu3(BTC)2:â€‰ An Effective Activation Procedure. Journal of Physical Chemistry C, 2007, 111, 9305-9313.	1.5	250
119	Simulation of Adsorption of DNA on Carbon Nanotubes. Journal of the American Chemical Society, 2007, 129, 10438-10445.	6.6	194
120	Polysulfone and functionalized carbon nanotube mixed matrix membranes for gas separation: Theory and experiment. Journal of Membrane Science, 2007, 294, 147-158.	4.1	346
121	Using first principles calculations to identify new destabilized metal hydride reactions for reversible hydrogen storage. Physical Chemistry Chemical Physics, 2007, 9, 1438.	1.3	173
122	Adsorption and diffusion of carbon dioxide and nitrogen through single-walled carbon nanotube membranes. Journal of Chemical Physics, 2006, 124, 054708.	1.2	175
123	Spectroscopic Measurement of Diffusion Kinetics through Subnanometer and Larger Al2O3Particles by a New Method:Â The Interaction of 2-Chloroethylethyl Sulfide with Î³-Al2O3. Journal of Physical Chemistry B, 2006, 110, 9204-9210.	1.2	11
124	First Principles Study of Adsorption and Dissociation of CO on W(111). Journal of Physical Chemistry B, 2006, 110, 1344-1349.	1.2	21
125	Identification of Destabilized Metal Hydrides for Hydrogen Storage Using First Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 8769-8776.	1.2	273
126	Transport Diffusion of Gases Is Rapid in Flexible Carbon Nanotubes. Journal of Physical Chemistry B, 2006, 110, 1971-1975.	1.2	146

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127	Quantum Sieving in Single-Walled Carbon Nanotubes:Â Effect of Interaction Potential and Rotationalâ^'Translational Coupling. Journal of Physical Chemistry B, 2006, 110, 1733-1741.	1.2	50
128	Unusual Hydrogen Bonding in Water-Filled Carbon Nanotubes. Journal of the American Chemical Society, 2006, 128, 12090-12097.	6.6	261
129	Direct observation of molecularly-aligned molecules in the second physisorbed layer-CO/Ag(110). Chemical Physics Letters, 2006, 418, 90-95.	1.2	4
130	Effects of an external electromagnetic field on rutile Tio2: A molecular dynamics study. Journal of Physics and Chemistry of Solids, 2006, 67, 1399-1409.	1.9	29
131	MATERIALS SCIENCE: Making High-Flux Membranes with Carbon Nanotubes. Science, 2006, 312, 1003-1004.	6.0	195
132	Molecular-dynamics simulations of methane hydrate dissociation. Journal of Chemical Physics, 2005, 123, 244503.	1.2	136
133	Formation of Odd-Numbered Clusters ofCO2Adsorbed on Nanotube Bundles. Physical Review Letters, 2005, 94, 125701.	2.9	31
134	Observation of a One-Dimensional Adsorption Site on Carbon Nanotubes:Â Adsorption of Alkanes of Different Molecular Lengths. Journal of Physical Chemistry B, 2005, 109, 20999-21005.	1.2	84
135	Dimensional Effects on the LOâ^'TO Splitting in CF4:Â First-Principles and Infrared Absorption Studies. Journal of the American Chemical Society, 2005, 127, 3198-3206.	6.6	12
136	An Effective Potential for Adsorption of Polar Molecules on Graphite. Molecular Simulation, 2005, 31, 1-10.	0.9	55
137	Adsorption of Gases in Metal Organic Materials:Â Comparison of Simulations and Experiments. Journal of Physical Chemistry B, 2005, 109, 13094-13103.	1.2	365
138	Oxygenated Hydrocarbon Ionic Surfactants Exhibit CO2Solubility. Journal of the American Chemical Society, 2005, 127, 11754-11762.	6.6	85
139	Surface tension of quantum fluids from molecular simulations. Journal of Chemical Physics, 2004, 120, 8707-8715.	1.2	11
140	Displacement ofCO2by Xe in single-walled carbon nanotube bundles. Physical Review B, 2004, 70, .	1.1	26
141	Vibrational behavior of adsorbed CO2 on single-walled carbon nanotubes. Journal of Chemical Physics, 2004, 120, 5377-5386.	1.2	73
142	Synthesis and Solubility of Linear Poly(tetrafluoroethylene-co-vinyl acetate) in Dense CO2:Â Experimental and Molecular Modeling Results. Macromolecules, 2004, 37, 7799-7807.	2.2	55
143	Wetting Transition of Water on Graphite and Other Surfaces. Journal of Physical Chemistry B, 2004, 108, 11704-11708.	1.2	42
144	Microporous Metal Organic Materials:Â Promising Candidates as Sorbents for Hydrogen Storage. Journal of the American Chemical Society, 2004, 126, 1308-1309.	6.6	615

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145	Diffusivities of Ar and Ne in Carbon Nanotubes. Molecular Simulation, 2003, 29, 677-684.	0.9	146
146	Chemical Activation of Single-Walled Carbon Nanotubes for Hydrogen Adsorption. Journal of Physical Chemistry B, 2003, 107, 3752-3760.	1.2	88
147	Trapped CO2in Carbon Nanotube Bundles. Journal of Physical Chemistry B, 2003, 107, 12930-12941.	1.2	94
148	Adsorption of CF4on the Internal and External Surfaces of Opened Single-Walled Carbon Nanotubes:Â A Vibrational Spectroscopy Study. Journal of the American Chemical Society, 2003, 125, 5889-5896.	6.6	108
149	Effect of Grafted Lewis Base Groups on the Phase Behavior of Model Poly(dimethyl siloxanes) in CO2. Industrial & Engineering Chemistry Research, 2003, 42, 6415-6424.	1.8	99
150	Gas Adsorption on Heterogeneous Single-Walled Carbon Nanotube Bundles. Physical Review Letters, 2003, 91, 015504.	2.9	149
151	Wetting transitions of hydrogen and deuterium on the surface of alkali metals. Physical Review B, 2003, 68, .	1.1	20
152	Adsorption and separation of hydrogen isotopes in carbon nanotubes: Multicomponent grand canonical Monte Carlo simulations. Journal of Chemical Physics, 2002, 116, 814-824.	1.2	172
153	Combined Experimental and Theoretical Investigation of Polar Organic Adsorption/Desorption from Model Carbonaceous Surfaces:Â Acetone on Graphite. Langmuir, 2002, 18, 2595-2600.	1.6	21
154	Rapid Transport of Gases in Carbon Nanotubes. Physical Review Letters, 2002, 89, 185901.	2.9	627
155	Igniting Nanotubes with a Flash. Science, 2002, 297, 192-193.	6.0	43
156	Phase transitions of adsorbed fluids computed from multiple-histogram reweighting. Molecular Physics, 2002, 100, 2139-2150.	0.8	41
157	Effect of confinement by porous materials on chemical reaction kinetics. Journal of Chemical Physics, 2002, 116, 2138-2148.	1.2	67
158	Layering and orientational ordering of propane on graphite: An experimental and simulation study. Journal of Chemical Physics, 2002, 117, 7719-7731.	1.2	23
159	Hydrogen storage in carbon nanotubes and graphitic nanofibers. Journal of Alloys and Compounds, 2002, 330-332, 659-665.	2.8	77
160	Effect of confinement on chemical reaction equilibria: The reactions 2NOâ‡”(NO)2 and N2+3H2â‡”2NH3 in carbon micropores. Journal of Chemical Physics, 2001, 114, 1851-1859.	1.2	106
161	Molecular simulation of xenon adsorption on single-walled carbon nanotubes. Journal of Chemical Physics, 2001, 114, 4180-4185.	1.2	122
162	Histogram reweighting and finite-size scaling study of the Lennardâ€“Jones fluids. Fluid Phase Equilibria, 2001, 187-188, 171-191.	1.4	68

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163	Optimization of Xe adsorption kinetics in single walled carbon nanotubes. Journal of Chemical Physics, 2001, 115, 6691-6698.	1.2	65
164	Light isotope separation in carbon nanotubes through quantum molecular sieving. Physical Review B, 2001, 63, .	1.1	100
165	An interatomic potential for mercury dimer. Journal of Chemical Physics, 2001, 114, 5545-5551.	1.2	47
166	Many-body interactions among adsorbed atoms and molecules within carbon nanotubes and in free space. Chemical Physics Letters, 2000, 332, 26-34.	1.2	48
167	Axial Phase of Quantum Fluids in Nanotubes. Journal of Low Temperature Physics, 2000, 120, 337-359.	0.6	39
168	An accurate H2â€“H2 interaction potential from first principles. Journal of Chemical Physics, 2000, 112, 4465-4473.	1.2	188
169	Molar excess volumes of liquid hydrogen and neon mixtures from path integral simulation. Journal of Chemical Physics, 1999, 111, 724-729.	1.2	8
170	Molecular simulation of hydrogen adsorption in charged single-walled carbon nanotubes. Journal of Chemical Physics, 1999, 111, 9778-9783.	1.2	145
171	Molecular simulation of hydrogen adsorption in single-walled carbon nanotubes and idealized carbon slit pores. Journal of Chemical Physics, 1999, 110, 577-586.	1.2	512
172	Computer Simulations of Hydrogen Adsorption on Graphite Nanofibers. Journal of Physical Chemistry B, 1999, 103, 277-281.	1.2	135
173	Quantum Sieving in Carbon Nanotubes and Zeolites. Physical Review Letters, 1999, 82, 956-959.	2.9	247
174	Optimization of Carbon Nanotube Arrays for Hydrogen Adsorption. Journal of Physical Chemistry B, 1999, 103, 4809-4813.	1.2	203
175	Computer Simulation Studies of Adsorption of Simple Gases on Alkali Metal Surfaces. Journal of Low Temperature Physics, 1998, 110, 653-658.	0.6	15
176	Adsorption of Hydrogen in Graphitic Slit Pores. International Journal of Thermophysics, 1998, 19, 835-844.	1.0	7
177	CO2â^'Fluorocarbon and CO2â^'Hydrocarbon Interactions from First-Principles Calculations. Journal of Physical Chemistry A, 1998, 102, 2231-2236.	1.1	107
178	Hydrogen adsorption on graphite and in carbon slit pores from path integral simulations. Molecular Physics, 1998, 95, 299-309.	0.8	81
179	Path integral grand canonical Monte Carlo. Journal of Chemical Physics, 1997, 107, 5108-5117.	1.2	92
180	C60sphase diagram: A full free-energy analysis. Physical Review B, 1997, 55, 2808-2817.	1.1	28

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181	Phase equilibrium of quantum fluids from simulation: Hydrogen and neon. Fluid Phase Equilibria, 1997, 132, 93-116.	1.4	60
182	Perturbation theory and computer simulations for linear and ring model polymers. Journal of Chemical Physics, 1996, 104, 1729-1742.	1.2	36
183	Equation of State for Lennard-Jones Chains. The Journal of Physical Chemistry, 1994, 98, 6413-6419.	2.9	237
184	Reactive canonical Monte Carlo. Molecular Physics, 1994, 81, 717-733.	0.8	191
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