J Karl Johnson

List of Publications by Citations

187 papers	13,054 citations	62 h-index	110 g-index
196 ext. papers	13,757 ext. citations	5 avg, IF	6.49 L-index

#	Paper	IF	Citations
187	The Lennard-Jones equation of state revisited. *Molecular Physics*, **1993**, 78, 591-618	1.7	1124
186	Microporous metal organic materials: promising candidates as sorbents for hydrogen storage. *Journal of the American Chemical Society*, **2004**, 126, 1308-9	16.4	581
185	Rapid transport of gases in carbon nanotubes. *Physical Review Letters*, **2002**, 89, 185901	7.4	568
184	Molecular simulation of hydrogen adsorption in single-walled carbon nanotubes and idealized carbon slit pores. *Journal of Chemical Physics*, **1999**, 110, 577-586	3.9	465
183	Adsorption of gases in metal organic materials: comparison of simulations and experiments. *Journal of Physical Chemistry B*, **2005**, 109, 13094-103	3.4	340
182	Polysulfone and functionalized carbon nanotube mixed matrix membranes for gas separation: Theory and experiment. *Journal of Membrane Science*, **2007**, 294, 147-158	9.6	310
181	Zwitterion functionalized carbon nanotube/polyamide nanocomposite membranes for water desalination. *ACS Nano*, **2013**, 7, 5308-19	16.7	289
180	Progress, Opportunities, and Challenges for Applying Atomically Detailed Modeling to Molecular Adsorption and Transport in Metal□Organic Framework Materials. *Industrial & Engineering Chemistry Research*, **2009**, 48, 2355-2371	3.9	270
179	Identification of destabilized metal hydrides for hydrogen storage using first principles calculations. *Journal of Physical Chemistry B*, **2006**, 110, 8769-76	3.4	249
178	Unusual hydrogen bonding in water-filled carbon nanotubes. *Journal of the American Chemical Society*, **2006**, 128, 12090-7	16.4	236
177	Quantum Sieving in Carbon Nanotubes and Zeolites. *Physical Review Letters*, **1999**, 82, 956-959	7.4	233
176	Experimental and Theoretical Studies of Gas Adsorption in Cu3(BTC)2: An Effective Activation Procedure. *Journal of Physical Chemistry C*, **2007**, 111, 9305-9313	3.8	232
175	Equation of State for Lennard-Jones Chains. *The Journal of Physical Chemistry*, **1994**, 98, 6413-6419		217
174	Optimization of Carbon Nanotube Arrays for Hydrogen Adsorption. *Journal of Physical Chemistry B*, **1999**, 103, 4809-4813	3.4	183
173	Materials science. Making high-flux membranes with carbon nanotubes. *Science*, **2006**, 312, 1003-4	33.3	179
172	Simulation of adsorption of DNA on carbon nanotubes. *Journal of the American Chemical Society*, **2007**, 129, 10438-45	16.4	178
171	Adsorption and separation of hydrogen isotopes in carbon nanotubes: Multicomponent grand canonical Monte Carlo simulations. *Journal of Chemical Physics*, **2002**, 116, 814-824	3.9	167

170	An accurate H2H2 interaction potential from first principles. *Journal of Chemical Physics*, **2000**, 112, 4465-4473	3.9	163
169	Using first principles calculations to identify new destabilized metal hydride reactions for reversible hydrogen storage. *Physical Chemistry Chemical Physics*, **2007**, 9, 1438-52	3.6	161
168	Adsorption and diffusion of carbon dioxide and nitrogen through single-walled carbon nanotube membranes. *Journal of Chemical Physics*, **2006**, 124, 054708	3.9	156
167	Reactive canonical Monte Carlo. *Molecular Physics*, **1994**, 81, 717-733	1.7	156
166	Systematic modulation and enhancement of CO2 : N2 selectivity and water stability in an isoreticular series of bio-MOF-11 analogues. *Chemical Science*, **2013**, 4, 1746	9.4	153
165	Gas adsorption on heterogeneous single-walled carbon nanotube bundles. *Physical Review Letters*, **2003**, 91, 015504	7.4	142
164	Diffusivities of Ar and Ne in Carbon Nanotubes. *Molecular Simulation*, **2003**, 29, 677-684	2	138
163	Transport diffusion of gases is rapid in flexible carbon nanotubes. *Journal of Physical Chemistry B*, **2006**, 110, 1971-5	3.4	135
162	Reaction mechanism of monoethanolamine with CO2 in aqueous solution from molecular modeling. *Journal of Physical Chemistry A*, **2010**, 114, 11844-52	2.8	130
161	Molecular simulation of hydrogen adsorption in charged single-walled carbon nanotubes. *Journal of Chemical Physics*, **1999**, 111, 9778-9783	3.9	128
160	Computer Simulations of Hydrogen Adsorption on Graphite Nanofibers. *Journal of Physical Chemistry B*, **1999**, 103, 277-281	3.4	120
159	Adsorption and Diffusion of Light Gases in ZIF-68 and ZIF-70: A Simulation Study. *Journal of Physical Chemistry C*, **2009**, 113, 16906-16914	3.8	118
158	Molecular simulation of xenon adsorption on single-walled carbon nanotubes. *Journal of Chemical Physics*, **2001**, 114, 4180-4185	3.9	116
157	Molecular-dynamics simulations of methane hydrate dissociation. *Journal of Chemical Physics*, **2005**, 123, 244503	3.9	114
156	Assessing nanoparticle size effects on metal hydride thermodynamics using the Wulff construction. *Nanotechnology*, **2009**, 20, 204001	3.4	113
155	Adsorption of CF4 on the internal and external surfaces of opened single-walled carbon nanotubes: a vibrational spectroscopy study. *Journal of the American Chemical Society*, **2003**, 125, 5889-96	16.4	103
154	Design of Lewis Pair-Functionalized Metal Organic Frameworks for CO2 Hydrogenation. *ACS Catalysis*, **2015**, 5, 2921-2928	13.1	102
153	Effect of confinement on chemical reaction equilibria: The reactions 2NO<=(NO)2 and N2+3H2<=2NH3 in carbon micropores. *Journal of Chemical Physics*, **2001**, 114, 1851-1859	3.9	101

152	CO2–Fluorocarbon and CO2–Hydrocarbon Interactions from First-Principles Calculations. *Journal of Physical Chemistry A*, **1998**, 102, 2231-2236	2.8	97
151	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	3.8	95
150	Large-Scale Screening of Metal Hydride Mixtures for High-Capacity Hydrogen Storage from First-Principles Calculations. *Journal of Physical Chemistry C*, **2008**, 112, 5258-5262	3.8	95
149	Light isotope separation in carbon nanotubes through quantum molecular sieving. *Physical Review B*, **2001**, 63,	3.3	93
148	Trapped CO2 in Carbon Nanotube Bundles. *Journal of Physical Chemistry B*, **2003**, 107, 12930-12941	3.4	91
147	Thermal conductivity of methane hydrate from experiment and molecular simulation. *Journal of Physical Chemistry B*, **2007**, 111, 13194-205	3.4	90
146	Simulation of chemical reaction equilibria by the reaction ensemble Monte Carlo method: a review. *Molecular Simulation*, **2008**, 34, 119-146	2	90
145	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	3.9	89
144	Atomically detailed models of gas mixture diffusion through CuBTC membranes. *Microporous and Mesoporous Materials*, **2009**, 125, 101-106	5.3	86
143	Adsorption and Diffusion of Hydrogen in a New Metal–Organic Framework Material: [Zn(bdc)(ted)0.5]. *Journal of Physical Chemistry C*, **2008**, 112, 2911-2917	3.8	85
142	Beyond Ordered Materials: Understanding Catalytic Sites on Amorphous Solids. *ACS Catalysis*, **2017**, 7, 7543-7557	13.1	84
141	Path integral grand canonical Monte Carlo. *Journal of Chemical Physics*, **1997**, 107, 5108-5117	3.9	84
140	Phase equilibria for associating Lennard-Jones fluids from theory and simulation. *Molecular Physics*, **1992**, 77, 1033-1053	1.7	84
139	Predicting Reaction Equilibria for Destabilized Metal Hydride Decomposition Reactions for Reversible Hydrogen Storage. *Journal of Physical Chemistry C*, **2007**, 111, 1584-1591	3.8	81
138	Phase Behavior of Oxygen-Containing Polymers in CO2. *Macromolecules*, **2007**, 40, 1332-1341	5.5	80
137	Observation of a one-dimensional adsorption site on carbon nanotubes: adsorption of alkanes of different molecular lengths. *Journal of Physical Chemistry B*, **2005**, 109, 20999-1005	3.4	79
136	Chemical Activation of Single-Walled Carbon Nanotubes for Hydrogen Adsorption. *Journal of Physical Chemistry B*, **2003**, 107, 3752-3760	3.4	79
135	Oxygenated hydrocarbon ionic surfactants exhibit CO2 solubility. *Journal of the American Chemical Society*, **2005**, 127, 11754-62	16.4	75

134	Hydrogen adsorption on graphite and in carbon slit pores from path integral simulations. *Molecular Physics*, **1998**, 95, 299-309	1.7	72
133	Accurate amorphous silica surface models from first-principles thermodynamics of surface dehydroxylation. *Langmuir*, **2014**, 30, 5133-41	4	69
132	Hydrogen storage in carbon nanotubes and graphitic nanofibers. *Journal of Alloys and Compounds*, **2002**, 330-332, 659-665	5.7	69
131	Vibrational behavior of adsorbed CO2 on single-walled carbon nanotubes. *Journal of Chemical Physics*, **2004**, 120, 5377-86	3.9	68
130	Histogram reweighting and finite-size scaling study of the Lennard□ones fluids. *Fluid Phase Equilibria*, **2001**, 187-188, 171-191	2.5	66
129	Design and evaluation of nonfluorous CO2-soluble oligomers and polymers. *Journal of Physical Chemistry B*, **2009**, 113, 14971-80	3.4	64
128	Testing the accuracy of correlations for multicomponent mass transport of adsorbed gases in metal-organic frameworks: diffusion of H2/CH4 mixtures in CuBTC. *Langmuir*, **2008**, 24, 8254-61	4	64
127	Effect of confinement by porous materials on chemical reaction kinetics. *Journal of Chemical Physics*, **2002**, 116, 2138-2148	3.9	64
126	Atomic charges derived from electrostatic potentials for molecular and periodic systems. *Journal of Physical Chemistry A*, **2010**, 114, 10225-33	2.8	62
125	CO2 capture properties of M□□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	3.3	62
124	Optimization of Xe adsorption kinetics in single walled carbon nanotubes. *Journal of Chemical Physics*, **2001**, 115, 6691-6698	3.9	62
123	Catalytic hydrogenation of CO2 to methanol in a Lewis pair functionalized MOF. *Catalysis Science and Technology*, **2016**, 6, 8392-8405	5.5	60
122	First-Principles Study of Experimental and Hypothetical Mg(BH4)2 Crystal Structures. *Journal of Physical Chemistry C*, **2008**, 112, 4391-4395	3.8	60
121	Screening Lewis Pair Moieties for Catalytic Hydrogenation of CO2 in Functionalized UiO-66. *ACS Catalysis*, **2015**, 5, 6219-6229	13.1	59
120	Phase equilibrium of quantum fluids from simulation: Hydrogen and neon. *Fluid Phase Equilibria*, **1997**, 132, 93-116	2.5	59
119	Porous Carbon Nanotube Membranes for Separation of H2/CH4 and CO2/CH4 Mixtures. *Journal of Physical Chemistry C*, **2012**, 116, 25904-25910	3.8	53
118	Aminosilicone solvents for CO(2) capture. *ChemSusChem*, **2010**, 3, 919-30	8.3	53
117	Solubility of CO2 in CO2-philic oligomers; COSMOtherm predictions and experimental results. *Fluid Phase Equilibria*, **2009**, 287, 26-32	2.5	52

116	Synthesis and Solubility of Linear Poly(tetrafluoroethylene-co-vinyl acetate) in Dense CO2: Experimental and Molecular Modeling Results. *Macromolecules*, **2004**, 37, 7799-7807	5.5	51
115	An Effective Potential for Adsorption of Polar Molecules on Graphite. *Molecular Simulation*, **2005**, 31, 1-10	2	50
114	Designing Open Metal Sites in Metal-Organic Frameworks for Paraffin/Olefin Separations. *Journal of the American Chemical Society*, **2019**, 141, 13003-13007	16.4	47
113	Adsorption of gases in carbon nanotubes: are defect interstitial sites important?. *Langmuir*, **2008**, 24, 9430-9	4	47
112	Quantum sieving in single-walled carbon nanotubes: effect of interaction potential and rotational-translational coupling. *Journal of Physical Chemistry B*, **2006**, 110, 1733-41	3.4	46
111	An interatomic potential for mercury dimer. *Journal of Chemical Physics*, **2001**, 114, 5545-5551	3.9	46
110	Effect of Support Preparation and Nanoparticle Size on Catalyst□Support Interactions between Pt and Amorphous Silica. *Journal of Physical Chemistry C*, **2015**, 119, 19934-19940	3.8	45
109	Hydrogen isotope separation in carbon nanotubes: calculation of coupled rotational and translational States at high densities. *ACS Nano*, **2010**, 4, 1703-15	16.7	43
108	Many-body interactions among adsorbed atoms and molecules within carbon nanotubes and in free space. *Chemical Physics Letters*, **2000**, 332, 26-34	2.5	43
107	Ozone Oxidation of Single Walled Carbon Nanotubes from Density Functional Theory. *Journal of Physical Chemistry C*, **2009**, 113, 17636-17642	3.8	42
106	Poly(vinyl acetate), poly((1-O-(vinyloxy) ethyl-2,3,4,6-tetra-O-acetyl-□d-glucopyranoside) and amorphous poly(lactic acid) are the most CO2-soluble oxygenated hydrocarbon-based polymers. *Journal of Supercritical Fluids*, **2008**, 46, 252-257	4.2	42
105	Critical Assessment of CO2Solubility in Volatile Solvents at 298.15 K. *Journal of Chemical & Engineering Data*, **2011**, 56, 1565-1572	2.8	41
104	Utilizing the Gate-Opening Mechanism in ZIF-7 for Adsorption Discrimination between N2O and CO2. *Journal of Physical Chemistry C*, **2014**, 118, 17831-17837	3.8	40
103	A computational study of the heats of reaction of substituted monoethanolamine with CO2. *Journal of Physical Chemistry A*, **2011**, 115, 342-50	2.8	40
102	The importance of charge□quadrupole interactions for H2 adsorption and diffusion in CuBTC. *Molecular Simulation*, **2009**, 35, 60-69	2	39
101	Wetting Transition of Water on Graphite and Other Surfaces. *Journal of Physical Chemistry B*, **2004**, 108, 11704-11708	3.4	39
100	Phase transitions of adsorbed fluids computed from multiple-histogram reweighting. *Molecular Physics*, **2002**, 100, 2139-2150	1.7	39
99	Igniting nanotubes with a flash. *Science*, **2002**, 297, 192-3; author reply 192-3	33.3	37

98	Influence of tert-amine groups on the solubility of polymers in CO2. *Polymer*, **2009**, 50, 2436-2444	3.9	36
97	Development of a ReaxFF reactive force field for tetrabutylphosphonium glycinate/CO2 mixtures. *Journal of Physical Chemistry B*, **2014**, 118, 12008-16	3.4	35
96	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	3.8	35
95	The role of van der Waals interactions in the adsorption of noble gases on metal surfaces. *Journal of Physics Condensed Matter*, **2012**, 24, 424211	1.8	35
94	Axial Phase of Quantum Fluids in Nanotubes. *Journal of Low Temperature Physics*, **2000**, 120, 337-359	1.3	35
93	Perturbation theory and computer simulations for linear and ring model polymers. *Journal of Chemical Physics*, **1996**, 104, 1729-1742	3.9	34
92	Development of a transferable reactive force field for cobalt. *Journal of Physical Chemistry A*, **2010**, 114, 5855-61	2.8	33
91	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	3.8	31
90	Noble gases on metal surfaces: Insights on adsorption site preference. *Physical Review B*, **2011**, 84,	3.3	30
89	First principles screening of destabilized metal hydrides for high capacity H2 storage using scandium. *Journal of Alloys and Compounds*, **2007**, 446-447, 23-27	5.7	30
88	Large-scale screening of metal hydrides for hydrogen storage from first-principles calculations based on equilibrium reaction thermodynamics. *Physical Chemistry Chemical Physics*, **2011**, 13, 7218-29	3.6	29
87	Structural and Electronic Properties of Pt13 Nanoclusters on Amorphous Silica Supports. *Journal of Physical Chemistry C*, **2015**, 119, 2503-2512	3.8	28
86	Formation of odd-numbered clusters of CO2 adsorbed on nanotube bundles. *Physical Review Letters*, **2005**, 94, 125701	7.4	28
85	First-Principles Characterization of Amorphous Phases of MB12H12, M = Mg, Ca. *Journal of Physical Chemistry C*, **2010**, 114, 14601-14605	3.8	26
84	C60sphase diagram: A full free-energy analysis. *Physical Review B*, **1997**, 55, 2808-2817	3.3	26
83	Vacancy clusters as entry ports for cesium intercalation in graphite. *Carbon*, **2011**, 49, 3937-3952	10.4	25
82	Stability analysis of doped materials for reversible hydrogen storage in destabilized metal hydrides. *Physical Review B*, **2007**, 76,	3.3	25
81	Shrinking Self-Interaction Errors with the Fermi-Löwdin Orbital Self-Interaction-Corrected Density Functional Approximation. *Journal of Physical Chemistry A*, **2018**, 122, 9307-9315	2.8	25

80	Displacement of CO2 by Xe in single-walled carbon nanotube bundles. *Physical Review B*, **2004**, 70,	3.3	24
79	Effects of an external electromagnetic field on rutile Tio2: A molecular dynamics study. *Journal of Physics and Chemistry of Solids*, **2006**, 67, 1399-1409	3.9	23
78	A first-principles study of lithium-decorated hybrid boron nitride and graphene domains for hydrogen storage. *Journal of Chemical Physics*, **2014**, 141, 084711	3.9	22
77	Tests of Pore-Size Distributions Deduced from Inversion of Simulated and Real Adsorption Data. *Journal of Low Temperature Physics*, **2009**, 157, 410-428	1.3	22
76	Design, Synthesis, and Characterization of Metal□Organic Frameworks for Enhanced Sorption of Chemical Warfare Agent Simulants. *Journal of Physical Chemistry C*, **2019**, 123, 19748-19758	3.8	21
75	Density functional theory study of CO2 capture with transition metal oxides and hydroxides. *Journal of Chemical Physics*, **2012**, 136, 064516	3.9	21
74	First principles study of adsorption and dissociation of CO on W(111). *Journal of Physical Chemistry B*, **2006**, 110, 1344-9	3.4	21
73	Experimental and theoretical comparison of gas desorption energies on metallic and semiconducting single-walled carbon nanotubes. *Journal of the American Chemical Society*, **2013**, 135, 7768-76	16.4	20
72	Prediction of CH4/H2 Mixture Selectivity in Zn(tbip) from Computer Simulations. *Journal of Low Temperature Physics*, **2009**, 157, 268-276	1.3	20
71	Wetting transitions of hydrogen and deuterium on the surface of alkali metals. *Physical Review B*, **2003**, 68,	3.3	20
70	Layering and orientational ordering of propane on graphite: An experimental and simulation study. *Journal of Chemical Physics*, **2002**, 117, 7719-7731	3.9	20
69	Impact of Support Interactions for Single-Atom Molybdenum Catalysts on Amorphous Silica. *Industrial & Engineering Chemistry Research*, **2016**, 55, 12350-12357	3.9	20
68	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	7.4	19
67	Combined Experimental and Theoretical Investigation of Polar Organic Adsorption/Desorption from Model Carbonaceous Surfaces: Acetone on Graphite. *Langmuir*, **2002**, 18, 2595-2600	4	19
66	Gas sorption properties of zwitterion-functionalized carbon nanotubes. *Journal of Membrane Science*, **2013**, 429, 88-94	9.6	18
65	First-Principles Investigation of Adsorption and Dissociation of Hydrogen on Mg2Si Surfaces. *Journal of Physical Chemistry C*, **2007**, 111, 6910-6916	3.8	18
64	Characterization of Bulk Structure in Zinc Orthotitanate: A Density Functional Theory and EXAFS Investigation. *Journal of the American Ceramic Society*, **2008**, 91, 584-590	3.8	17
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62	Reaction of the Basal Plane of Graphite with the Methyl Radical. *Journal of Physical Chemistry Letters*, **2012**, 3, 1680-3	6.4	16
61	Defect and Nondefect Interstitial Channel Availability in Carbon Nanotube Bundles: Comparison of Modeling with Experiments. *Journal of Physical Chemistry C*, **2010**, 114, 7602-7610	3.8	16
60	Inter- and Intratube Self-Diffusion in n-Heptane Adsorbed on Carbon Nanotubes. *Journal of Physical Chemistry C*, **2007**, 111, 4578-4584	3.8	16
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58	Energy Efficient Formaldehyde Synthesis by Direct Hydrogenation of Carbon Monoxide in Functionalized Metal□Organic Frameworks. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 2508-2515	8.3	16
57	Facile Anhydrous Proton Transport on Hydroxyl Functionalized Graphane. *Physical Review Letters*, **2017**, 118, 186101	7.4	15
56	Computer Simulation Studies of Adsorption of Simple Gases on Alkali Metal Surfaces. *Journal of Low Temperature Physics*, **1998**, 110, 653-658	1.3	15
55	Quantum chemistry benchmarking of binding and selectivity for lanthanide extractants. *International Journal of Quantum Chemistry*, **2018**, 118, e25516	2.1	14
54	Reactive Canonical Monte Carlo. *Advances in Chemical Physics*, **2007**, 461-481		14
53	Mechanism of Isobutylene Polymerization: Quantum Chemical Insight into AlCl3/H2O-Catalyzed Reactions. *ACS Catalysis*, **2018**, 8, 8006-8013	13.1	13
52	Methyl Radical Reactivity on the Basal Plane of Graphite. *Journal of Physical Chemistry C*, **2012**, 116, 18347-18357	3.8	12
51	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	3.8	12
50	A corresponding states principle for physisorption and deviations for quantum fluids. *Molecular Physics*, **2008**, 106, 1579-1585	1.7	12
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48	The effect of topology in Lewis pair functionalized metal organic frameworks on CO2 adsorption and hydrogenation. *Catalysis Science and Technology*, **2018**, 8, 4609-4617	5.5	11
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44	Toward Understanding the Kinetics of CO Capture on Sodium Carbonate. *ACS Applied Materials & Interfaces*, **2019**, 11, 9033-9041	9.5	10
43	Effect of Spin-Crossover-Induced Pore Contraction on CO2□Host Interactions in the Porous Coordination Polymers [Fe(pyrazine)M(CN)4] (M = Ni, Pt). *European Journal of Inorganic Chemistry*, **2013**, 2013, 511-519	2.3	10
42	Adsorbed Gases in Bundles of Carbon Nanotubes **2008**, 187-210		10
41	Spectroscopic measurement of diffusion kinetics through subnanometer and larger Al2O3 particles by a new method: the interaction of 2-chloroethylethyl sulfide with gamma-Al2O3. *Journal of Physical Chemistry B*, **2006**, 110, 9204-10	3.4	10
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38	Surface reactions of AsH3, H2Se, and H2S on the Zn2TiO4(010) surface. *Surface Science*, **2011**, 605, 818-823	2.3	9
37	Surface tension of quantum fluids from molecular simulations. *Journal of Chemical Physics*, **2004**, 120, 8707-15	3.9	9
36	H/CO separations in multicomponent metal-adeninate MOFs with multiple chemically distinct pore environments. *Chemical Science*, **2020**, 11, 12807-12815	9.4	9
35	Density functional theory studies on the electronic, structural, phonon dynamical and thermo-stability properties of bicarbonates MHCO(3), M□=□Li, Na, K. *Journal of Physics Condensed Matter*, **2012**, 24, 325501, 1-16	1.8	8
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33	Application of Self-Interaction Corrected Density Functional Theory to Early, Middle, and Late Transition States. *Journal of Physical Chemistry A*, **2020**, 124, 8223-8234	2.8	8
32	A Combined Experimental and Computational Study on Selected Physical Properties of Aminosilicones. *Industrial & Engineering Chemistry Research*, **2014**, 53, 1334-1341	3.9	7
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30	Unraveling Anhydrous Proton Conduction in Hydroxygraphane. *Journal of Physical Chemistry Letters* , **2019**, 10, 518-523	6.4	7
29	Cavity correlation and bridge functions at high density and near the critical point: a test of second-order Percus□evick theory. *Molecular Physics*, **2016**, 114, 2516-2522	1.7	6
28	Fundamental Insights into the Reactivity and Utilization of Open Metal Sites in Cu(I)-MFU-4l. *Organometallics*, **2019**, 38, 3453-3459	3.8	6
27	Adsorption of Hydrogen in Graphitic Slit Pores. *International Journal of Thermophysics*, **1998**, 19, 835-844	2.1	6

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23	Vibron hopping and bond anharmonicity in hot dense hydrogen. *Journal of Chemical Physics*, **2009**, 130, 054502	3.9	5
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20	Study of self-interaction-errors in barrier heights using locally scaled and Perdew-Zunger self-interaction methods.. *Journal of Chemical Physics*, **2022**, 156, 014306	3.9	5
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18	Direct observation of molecularly-aligned molecules in the second physisorbed layer-CO/Ag(1 1 0). *Chemical Physics Letters*, **2006**, 418, 90-95	2.5	4
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