

J Karl Johnson

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Study of self-interaction-errors in barrier heights using locally scaled and Perdew-Zunger self-interaction methods.. <i>Journal of Chemical Physics</i> , 2022 , 156, 014306	3.9	5
186	Effect of Chain Length on the Dipole Moment of Polyisobutylene Succinate Anhydride. <i>Industrial & Engineering Chemistry Research</i> , 2022 , 61, 2359-2365	3.9	0
185	Fermi-L�wdin orbital self-interaction correction of adsorption energies on transition metal ions.. <i>Journal of Chemical Physics</i> , 2022 , 156, 134102	3.9	1
184	Theoretical Study of the Impact of Vacancies and Disorder on the Electronic Properties of Cu ₂ Se. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 12324-12332	3.8	1
183	Binding of CO and O on Low-Symmetry Pt Clusters Supported on Amorphous Silica. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 13780-13787	3.8	1
182	Efficiently Trained Deep Learning Potential for Graphane. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 14874-14882	3.8	2
181	In Situ Nuclear Magnetic Resonance Investigation of Molecular Adsorption and Kinetics in Metal-Organic Framework UiO-66. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 892-899	6.4	3
180	Adsorption separation of heavier isotope gases in subnanometer carbon pores. <i>Nature Communications</i> , 2021 , 12, 546	17.4	6
179	Impact of defects on the decomposition of chemical warfare agent simulants in Zr-based metal organic frameworks. <i>AIChE Journal</i> , 2021 , 67, e17156	3.6	1
178	H/CO separations in multicomponent metal-adeninate MOFs with multiple chemically distinct pore environments. <i>Chemical Science</i> , 2020 , 11, 12807-12815	9.4	9
177	Understanding and Improving the Kinetics of Bulk Carbonation on Sodium Carbonate. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 23106-23115	3.8	1
176	Application of Self-Interaction Corrected Density Functional Theory to Early, Middle, and Late Transition States. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 8223-8234	2.8	8
175	Modeling of Diffusion of Acetone in UiO-66. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 28469-28478	3.8	10
174	Test of the Duh-Haymet-Henderson theory for mixtures: cavity correlation functions and excess volumes. <i>Molecular Physics</i> , 2019 , 117, 3623-3631	1.7	
173	Toward Understanding the Kinetics of CO Capture on Sodium Carbonate. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 9033-9041	9.5	10
172	Design, Synthesis, and Characterization of Metal-Organic Frameworks for Enhanced Sorption of Chemical Warfare Agent Simulants. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 19748-19758	3.8	21
171	Designing Open Metal Sites in Metal-Organic Frameworks for Paraffin/Olefin Separations. <i>Journal of the American Chemical Society</i> , 2019 , 141, 13003-13007	16.4	47

170	Fundamental Insights into the Reactivity and Utilization of Open Metal Sites in Cu(I)-MFU-4L. <i>Organometallics</i> , 2019 , 38, 3453-3459	3.8	6
169	Method for Predicting Dipole Moments of Complex Molecules for Use in Thermophysical Property Estimation. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 19263-19270	3.9	3
168	Graphamine: Amine-Functionalized Graphane for Intrinsic Anhydrous Proton Conduction. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 1566-1571	3.8	7
167	Energy Efficient Formaldehyde Synthesis by Direct Hydrogenation of Carbon Monoxide in Functionalized Metal-Organic Frameworks. <i>ACS Sustainable Chemistry and Engineering</i> , 2019 , 7, 2508-2515	8.3	16
166	Unraveling Anhydrous Proton Conduction in Hydroxygraphane. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 518-523	6.4	7
165	Quantum chemistry benchmarking of binding and selectivity for lanthanide extractants. <i>International Journal of Quantum Chemistry</i> , 2018 , 118, e25516	2.1	14
164	Mechanism of Isobutylene Polymerization: Quantum Chemical Insight into AlCl ₃ /H ₂ O-Catalyzed Reactions. <i>ACS Catalysis</i> , 2018 , 8, 8006-8013	13.1	13
163	The effect of topology in Lewis pair functionalized metal organic frameworks on CO ₂ adsorption and hydrogenation. <i>Catalysis Science and Technology</i> , 2018 , 8, 4609-4617	5.5	11
162	Shrinking Self-Interaction Errors with the Fermi-Löwdin Orbital Self-Interaction-Corrected Density Functional Approximation. <i>Journal of Physical Chemistry A</i> , 2018 , 122, 9307-9315	2.8	25
161	TiH ₂ as a Dynamic Additive for Improving the De/Rehydrogenation Properties of MgH ₂ : A Combined Experimental and Theoretical Mechanistic Investigation. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 21248-21261	3.8	31
160	Screening the activity of Lewis pairs for hydrogenation of CO ₂ . <i>Molecular Simulation</i> , 2017 , 43, 821-827	2	11
159	A comparison of the correlation functions of the Lennard-Jones fluid for the first-order Duhem-Blaynet-Blenderson closure with molecular simulations. <i>Molecular Physics</i> , 2017 , 115, 1335-1342	1.7	2
158	Adsorption and Diffusion of Fluids in Defective Carbon Nanotubes: Insights from Molecular Simulations. <i>Langmuir</i> , 2017 , 33, 11834-11844	4	5
157	Beyond Ordered Materials: Understanding Catalytic Sites on Amorphous Solids. <i>ACS Catalysis</i> , 2017 , 7, 7543-7557	13.1	84
156	Facile Anhydrous Proton Transport on Hydroxyl Functionalized Graphane. <i>Physical Review Letters</i> , 2017 , 118, 186101	7.4	15
155	Catalytic hydrogenation of CO ₂ to methanol in a Lewis pair functionalized MOF. <i>Catalysis Science and Technology</i> , 2016 , 6, 8392-8405	5.5	60
154	Cavity correlation and bridge functions at high density and near the critical point: a test of second-order Percus-Yevick theory. <i>Molecular Physics</i> , 2016 , 114, 2516-2522	1.7	6
153	Impact of Support Interactions for Single-Atom Molybdenum Catalysts on Amorphous Silica. <i>Industrial & Engineering Chemistry Research</i> , 2016 , 55, 12350-12357	3.9	20

152	Predicting catalyst-support interactions between metal nanoparticles and amorphous silica supports. <i>Surface Science</i> , 2016 , 652, 278-285	1.8	16
151	Design of Lewis Pair-Functionalized Metal Organic Frameworks for CO ₂ Hydrogenation. <i>ACS Catalysis</i> , 2015 , 5, 2921-2928	13.1	102
150	Screening Lewis Pair Moieties for Catalytic Hydrogenation of CO ₂ in Functionalized UiO-66. <i>ACS Catalysis</i> , 2015 , 5, 6219-6229	13.1	59
149	Effect of Support Preparation and Nanoparticle Size on Catalyst-Support Interactions between Pt and Amorphous Silica. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 19934-19940	3.8	45
148	Structural and Electronic Properties of Pt ₁₃ Nanoclusters on Amorphous Silica Supports. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 2503-2512	3.8	28
147	Accurate amorphous silica surface models from first-principles thermodynamics of surface dehydroxylation. <i>Langmuir</i> , 2014 , 30, 5133-41	4	69
146	Utilizing the Gate-Opening Mechanism in ZIF-7 for Adsorption Discrimination between N ₂ O and CO ₂ . <i>Journal of Physical Chemistry C</i> , 2014 , 118, 17831-17837	3.8	40
145	Development of a ReaxFF reactive force field for tetrabutylphosphonium glycinate/CO ₂ mixtures. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 12008-16	3.4	35
144	Elucidation of Aqueous Solvent-Mediated Hydrogen-Transfer Reactions by ab Initio Molecular Dynamics and Nudged Elastic-Band Studies of NaBH ₄ Hydrolysis. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 21385-21399	3.8	35
143	A Combined Experimental and Computational Study on Selected Physical Properties of Aminosilicones. <i>Industrial & Engineering Chemistry Research</i> , 2014 , 53, 1334-1341	3.9	7
142	A first-principles study of lithium-decorated hybrid boron nitride and graphene domains for hydrogen storage. <i>Journal of Chemical Physics</i> , 2014 , 141, 084711	3.9	22
141	Deliquescence of NaBH ₄ from Density Functional Theory and Experiments. <i>Industrial & Engineering Chemistry Research</i> , 2013 , 52, 13849-13861	3.9	3
140	Effect of Spin-Crossover-Induced Pore Contraction on CO ₂ -Host Interactions in the Porous Coordination Polymers [Fe(pyrazine)M(CN) ₄] (M = Ni, Pt). <i>European Journal of Inorganic Chemistry</i> , 2013 , 2013, 511-519	2.3	10
139	Gas sorption properties of zwitterion-functionalized carbon nanotubes. <i>Journal of Membrane Science</i> , 2013 , 429, 88-94	9.6	18
138	Systematic modulation and enhancement of CO ₂ : N ₂ selectivity and water stability in an isorecticular series of bio-MOF-11 analogues. <i>Chemical Science</i> , 2013 , 4, 1746	9.4	153
137	Is there a difference in van der Waals interactions between rare gas atoms adsorbed on metallic and semiconducting single-walled carbon nanotubes?. <i>Physical Review Letters</i> , 2013 , 110, 135503	7.4	19
136	Experimental and theoretical comparison of gas desorption energies on metallic and semiconducting single-walled carbon nanotubes. <i>Journal of the American Chemical Society</i> , 2013 , 135, 7768-76	16.4	20
135	Zwitterion functionalized carbon nanotube/polyamide nanocomposite membranes for water desalination. <i>ACS Nano</i> , 2013 , 7, 5308-19	16.7	289

134	Properties of Weakly Bound Molecular Oxygen on the Rutile TiO ₂ (110) Surface from Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 17151-17158	3.8	2
133	Porous Carbon Nanotube Membranes for Separation of H ₂ /CH ₄ and CO ₂ /CH ₄ Mixtures. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 25904-25910	3.8	53
132	Density functional theory studies on the electronic, structural, phonon dynamical and thermo-stability properties of bicarbonates MHCO ₃ , M=Li, Na, K. <i>Journal of Physics Condensed Matter</i> , 2012 , 24, 325501, 1-16	1.8	8
131	Methyl Radical Reactivity on the Basal Plane of Graphite. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 18347-18357	3.7	17
130	Density functional theory study of CO ₂ capture with transition metal oxides and hydroxides. <i>Journal of Chemical Physics</i> , 2012 , 136, 064516	3.9	21
129	The role of van der Waals interactions in the adsorption of noble gases on metal surfaces. <i>Journal of Physics Condensed Matter</i> , 2012 , 24, 424211	1.8	35
128	Reaction of the Basal Plane of Graphite with the Methyl Radical. <i>Journal of Physical Chemistry Letters</i> , 2012 , 3, 1680-3	6.4	16
127	Molecular Simulations and Theoretical Predictions for Adsorption and Diffusion of CH ₄ /H ₂ and CO ₂ /CH ₄ Mixtures in ZIFs. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 12560-12566	3.8	95
126	Methyl Chloride Reactions on Lithiated Carbon Nanotubes: Lithium as Both Reactant and Catalyst. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 11694-11700	3.8	8
125	Large-scale screening of metal hydrides for hydrogen storage from first-principles calculations based on equilibrium reaction thermodynamics. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 7218-29	3.6	29
124	Examining the robustness of first-principles calculations for metal hydride reaction thermodynamics by detection of metastable reaction pathways. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 21520-9	3.6	11
123	A computational study of the heats of reaction of substituted monoethanolamine with CO ₂ . <i>Journal of Physical Chemistry A</i> , 2011 , 115, 342-50	2.8	40
122	Critical Assessment of CO ₂ Solubility in Volatile Solvents at 298.15 K. <i>Journal of Chemical & Engineering Data</i> , 2011 , 56, 1565-1572	2.8	41
121	Vacancy clusters as entry ports for cesium intercalation in graphite. <i>Carbon</i> , 2011 , 49, 3937-3952	10.4	25
120	CO ₂ capture properties of MCO ₃ H (M=Li, Na, K) systems: A combined density functional theory and lattice phonon dynamics study. <i>Journal of Solid State Chemistry</i> , 2011 , 184, 304-311	3.3	62
119	Surface reactions of AsH ₃ , H ₂ Se, and H ₂ S on the Zn ₂ TiO ₄ (010) surface. <i>Surface Science</i> , 2011 , 605, 818-823	3.2	9
118	Noble gases on metal surfaces: Insights on adsorption site preference. <i>Physical Review B</i> , 2011 , 84,	3.3	30
117	One-dimensional adsorption and diffusion in Zn(tbp). <i>Molecular Simulation</i> , 2011 , 37, 640-646	2	5

116	First principles study of vacancy and tungsten diffusion in fcc cobalt. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2010 , 18, 015008	2	11
115	Development of a transferable reactive force field for cobalt. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 5855-61	2.8	33
114	First-Principles Characterization of Amorphous Phases of MB ₁₂ H ₁₂ , M = Mg, Ca. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 14601-14605	3.8	26
113	Defect and Nondefect Interstitial Channel Availability in Carbon Nanotube Bundles: Comparison of Modeling with Experiments. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 7602-7610	3.8	16
112	Hydrogen isotope separation in carbon nanotubes: calculation of coupled rotational and translational States at high densities. <i>ACS Nano</i> , 2010 , 4, 1703-15	16.7	43
111	Reaction mechanism of monoethanolamine with CO ₂ in aqueous solution from molecular modeling. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 11844-52	2.8	130
110	Carbon-Chlorine Bond Scission in Li-Doped Single-Walled Carbon Nanotubes: Reaction of CH ₃ Cl and Lithium. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 17148-17158	3.8	9
109	Atomic charges derived from electrostatic potentials for molecular and periodic systems. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 10225-33	2.8	62
108	Aminosilicone solvents for CO ₂ capture. <i>ChemSusChem</i> , 2010 , 3, 919-30	8.3	53
107	Vibron hopping and bond anharmonicity in hot dense hydrogen. <i>Journal of Chemical Physics</i> , 2009 , 130, 054502	3.9	5
106	Assessing nanoparticle size effects on metal hydride thermodynamics using the Wulff construction. <i>Nanotechnology</i> , 2009 , 20, 204001	3.4	113
105	Solubility of CO ₂ in CO ₂ -philic oligomers; COSMOtherm predictions and experimental results. <i>Fluid Phase Equilibria</i> , 2009 , 287, 26-32	2.5	52
104	Prediction of CH ₄ /H ₂ Mixture Selectivity in Zn(tbip) from Computer Simulations. <i>Journal of Low Temperature Physics</i> , 2009 , 157, 268-276	1.3	20
103	Tests of Pore-Size Distributions Deduced from Inversion of Simulated and Real Adsorption Data. <i>Journal of Low Temperature Physics</i> , 2009 , 157, 410-428	1.3	22
102	Atomically detailed models of gas mixture diffusion through CuBTC membranes. <i>Microporous and Mesoporous Materials</i> , 2009 , 125, 101-106	5.3	86
101	Influence of tert-amine groups on the solubility of polymers in CO ₂ . <i>Polymer</i> , 2009 , 50, 2436-2444	3.9	36
100	Enhancement of Adsorption Inside Single-Walled Carbon Nanotubes: Li Doping Effect on n-Heptane van der Waals Bonding. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 4829-4838	3.8	12
99	Adsorption and Diffusion of Light Gases in ZIF-68 and ZIF-70: A Simulation Study. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 16906-16914	3.8	118

98	Ozone Oxidation of Single Walled Carbon Nanotubes from Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 17636-17642	3.8	42
97	The importance of charge-quadrupole interactions for H ₂ adsorption and diffusion in CuBTC. <i>Molecular Simulation</i> , 2009 , 35, 60-69	2	39
96	Progress, Opportunities, and Challenges for Applying Atomically Detailed Modeling to Molecular Adsorption and Transport in Metal-Organic Framework Materials. <i>Industrial & Engineering Chemistry Research</i> , 2009 , 48, 2355-2371	3.9	270
95	Design and evaluation of nonfluorous CO ₂ -soluble oligomers and polymers. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 14971-80	3.4	64
94	Adsorption and Diffusion of Hydrogen in a New Metal-Organic Framework Material: [Zn(bdc)(ted) _{0.5}]. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 2911-2917	3.8	85
93	Large-Scale Screening of Metal Hydride Mixtures for High-Capacity Hydrogen Storage from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 5258-5262	3.8	95
92	Influence of Surface Reactions on Complex Hydride Reversibility. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 18270-18279	3.8	4
91	First-Principles Study of Experimental and Hypothetical Mg(BH ₄) ₂ Crystal Structures. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 4391-4395	3.8	60
90	Testing the accuracy of correlations for multicomponent mass transport of adsorbed gases in metal-organic frameworks: diffusion of H ₂ /CH ₄ mixtures in CuBTC. <i>Langmuir</i> , 2008 , 24, 8254-61	4	64
89	Adsorbed Gases in Bundles of Carbon Nanotubes 2008 , 187-210		10
88	Hydrogen Adsorption in Single-Walled Carbon Nanotubes 2008 , 369-401		1
87	Adsorption of gases in carbon nanotubes: are defect interstitial sites important?. <i>Langmuir</i> , 2008 , 24, 9430-9	4	47
86	Density functional theory calculations of the surface structure of the inverse spinel zinc orthotitanate. <i>Journal of Physics Condensed Matter</i> , 2008 , 20, 095001	1.8	3
85	A corresponding states principle for physisorption and deviations for quantum fluids. <i>Molecular Physics</i> , 2008 , 106, 1579-1585	1.7	12
84	DFT characterization of adsorption and diffusion mechanisms of H, As, S, and Se on the zinc orthotitanate(0 1 0) surface. <i>Surface Science</i> , 2008 , 602, 1877-1882	1.8	2
83	Poly(vinyl acetate), poly((1-O-(vinyl-2,3,4,6-tetra-O-acetyl- β -D-glucopyranoside) and amorphous poly(lactic acid) are the most CO ₂ -soluble oxygenated hydrocarbon-based polymers. <i>Journal of Supercritical Fluids</i> , 2008 , 46, 252-257	4.2	42
82	Simulation of chemical reaction equilibria by the reaction ensemble Monte Carlo method: a review \square <i>Molecular Simulation</i> , 2008 , 34, 119-146	2	90
81	Characterization of Bulk Structure in Zinc Orthotitanate: A Density Functional Theory and EXAFS Investigation. <i>Journal of the American Ceramic Society</i> , 2008 , 91, 584-590	3.8	17

80	First-Principles Investigation of Adsorption and Dissociation of Hydrogen on Mg ₂ Si Surfaces. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 6910-6916	3.8	18
79	Predicting Reaction Equilibria for Destabilized Metal Hydride Decomposition Reactions for Reversible Hydrogen Storage. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 1584-1591	3.8	81
78	Inter- and Intratube Self-Diffusion in n-Heptane Adsorbed on Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 4578-4584	3.8	16
77	Thermal conductivity of methane hydrate from experiment and molecular simulation. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 13194-205	3.4	90
76	Experimental and Theoretical Studies of Gas Adsorption in Cu ₃ (BTC) ₂ : An Effective Activation Procedure. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 9305-9313	3.8	232
75	Simulation of adsorption of DNA on carbon nanotubes. <i>Journal of the American Chemical Society</i> , 2007 , 129, 10438-45	16.4	178
74	Polysulfone and functionalized carbon nanotube mixed matrix membranes for gas separation: Theory and experiment. <i>Journal of Membrane Science</i> , 2007 , 294, 147-158	9.6	310
73	Using first principles calculations to identify new destabilized metal hydride reactions for reversible hydrogen storage. <i>Physical Chemistry Chemical Physics</i> , 2007 , 9, 1438-52	3.6	161
72	Reactive Canonical Monte Carlo. <i>Advances in Chemical Physics</i> , 2007 , 461-481		14
71	Phase Behavior of Oxygen-Containing Polymers in CO ₂ . <i>Macromolecules</i> , 2007 , 40, 1332-1341	5.5	80
70	First principles screening of destabilized metal hydrides for high capacity H ₂ storage using scandium. <i>Journal of Alloys and Compounds</i> , 2007 , 446-447, 23-27	5.7	30
69	Stability analysis of doped materials for reversible hydrogen storage in destabilized metal hydrides. <i>Physical Review B</i> , 2007 , 76,	3.3	25
68	Materials science. Making high-flux membranes with carbon nanotubes. <i>Science</i> , 2006 , 312, 1003-4	33.3	179
67	Adsorption and diffusion of carbon dioxide and nitrogen through single-walled carbon nanotube membranes. <i>Journal of Chemical Physics</i> , 2006 , 124, 054708	3.9	156
66	Spectroscopic measurement of diffusion kinetics through subnanometer and larger Al ₂ O ₃ particles by a new method: the interaction of 2-chloroethylethyl sulfide with gamma-Al ₂ O ₃ . <i>Journal of Physical Chemistry B</i> , 2006 , 110, 9204-10	3.4	10
65	First principles study of adsorption and dissociation of CO on W(111). <i>Journal of Physical Chemistry B</i> , 2006 , 110, 1344-9	3.4	21
64	Identification of destabilized metal hydrides for hydrogen storage using first principles calculations. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 8769-76	3.4	249
63	Transport diffusion of gases is rapid in flexible carbon nanotubes. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 1971-5	3.4	135

62	Quantum sieving in single-walled carbon nanotubes: effect of interaction potential and rotational-translational coupling. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 1733-41	3.4	46
61	Unusual hydrogen bonding in water-filled carbon nanotubes. <i>Journal of the American Chemical Society</i> , 2006 , 128, 12090-7	16.4	236
60	Direct observation of molecularly-aligned molecules in the second physisorbed layer-CO/Ag(1 1 0). <i>Chemical Physics Letters</i> , 2006 , 418, 90-95	2.5	4
59	Effects of an external electromagnetic field on rutile TiO ₂ : A molecular dynamics study. <i>Journal of Physics and Chemistry of Solids</i> , 2006 , 67, 1399-1409	3.9	23
58	Observation of a one-dimensional adsorption site on carbon nanotubes: adsorption of alkanes of different molecular lengths. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 20999-1005	3.4	79
57	Dimensional effects on the LO-TO splitting in CF ₄ : first-principles and infrared absorption studies. <i>Journal of the American Chemical Society</i> , 2005 , 127, 3198-206	16.4	11
56	An Effective Potential for Adsorption of Polar Molecules on Graphite. <i>Molecular Simulation</i> , 2005 , 31, 1-10	2	50
55	Adsorption of gases in metal organic materials: comparison of simulations and experiments. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 13094-103	3.4	34 ^o
54	Oxygenated hydrocarbon ionic surfactants exhibit CO ₂ solubility. <i>Journal of the American Chemical Society</i> , 2005 , 127, 11754-62	16.4	75
53	Molecular-dynamics simulations of methane hydrate dissociation. <i>Journal of Chemical Physics</i> , 2005 , 123, 244503	3.9	114
52	Formation of odd-numbered clusters of CO ₂ adsorbed on nanotube bundles. <i>Physical Review Letters</i> , 2005 , 94, 125701	7.4	28
51	Surface tension of quantum fluids from molecular simulations. <i>Journal of Chemical Physics</i> , 2004 , 120, 8707-15	3.9	9
50	Displacement of CO ₂ by Xe in single-walled carbon nanotube bundles. <i>Physical Review B</i> , 2004 , 70,	3.3	24
49	Vibrational behavior of adsorbed CO ₂ on single-walled carbon nanotubes. <i>Journal of Chemical Physics</i> , 2004 , 120, 5377-86	3.9	68
48	Synthesis and Solubility of Linear Poly(tetrafluoroethylene-co-vinyl acetate) in Dense CO ₂ : Experimental and Molecular Modeling Results. <i>Macromolecules</i> , 2004 , 37, 7799-7807	5.5	51
47	Wetting Transition of Water on Graphite and Other Surfaces. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 11704-11708	3.4	39
46	Microporous metal organic materials: promising candidates as sorbents for hydrogen storage. <i>Journal of the American Chemical Society</i> , 2004 , 126, 1308-9	16.4	58 ¹
45	Diffusivities of Ar and Ne in Carbon Nanotubes. <i>Molecular Simulation</i> , 2003 , 29, 677-684	2	138

44	Chemical Activation of Single-Walled Carbon Nanotubes for Hydrogen Adsorption. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 3752-3760	3.4	79
43	Trapped CO ₂ in Carbon Nanotube Bundles. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 12930-12941	3.4	91
42	Adsorption of CF ₄ on the internal and external surfaces of opened single-walled carbon nanotubes: a vibrational spectroscopy study. <i>Journal of the American Chemical Society</i> , 2003 , 125, 5889-96	16.4	103
41	Effect of Grafted Lewis Base Groups on the Phase Behavior of Model Poly(dimethyl siloxanes) in CO ₂ . <i>Industrial & Engineering Chemistry Research</i> , 2003 , 42, 6415-6424	3.9	89
40	Gas adsorption on heterogeneous single-walled carbon nanotube bundles. <i>Physical Review Letters</i> , 2003 , 91, 015504	7.4	142
39	Wetting transitions of hydrogen and deuterium on the surface of alkali metals. <i>Physical Review B</i> , 2003 , 68,	3.3	20
38	Adsorption and separation of hydrogen isotopes in carbon nanotubes: Multicomponent grand canonical Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 2002 , 116, 814-824	3.9	167
37	Combined Experimental and Theoretical Investigation of Polar Organic Adsorption/Desorption from Model Carbonaceous Surfaces: Acetone on Graphite. <i>Langmuir</i> , 2002 , 18, 2595-2600	4	19
36	Rapid transport of gases in carbon nanotubes. <i>Physical Review Letters</i> , 2002 , 89, 185901	7.4	568
35	Igniting nanotubes with a flash. <i>Science</i> , 2002 , 297, 192-3; author reply 192-3	33.3	37
34	Phase transitions of adsorbed fluids computed from multiple-histogram reweighting. <i>Molecular Physics</i> , 2002 , 100, 2139-2150	1.7	39
33	Effect of confinement by porous materials on chemical reaction kinetics. <i>Journal of Chemical Physics</i> , 2002 , 116, 2138-2148	3.9	64
32	Layering and orientational ordering of propane on graphite: An experimental and simulation study. <i>Journal of Chemical Physics</i> , 2002 , 117, 7719-7731	3.9	20
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23	Axial Phase of Quantum Fluids in Nanotubes. <i>Journal of Low Temperature Physics</i> , 2000 , 120, 337-359	1.3	35
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