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	The Lennard-Jones equation of state revisited. Molecular Physics, 1993, 78, 591-618.	0.8	1,245
2	Rapid Transport of Gases in Carbon Nanotubes. Physical Review Letters, 2002, 89, 185901.	2.9	627
3	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
4	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
5	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
6	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
7	Zwitterion Functionalized Carbon Nanotube/Polyamide Nanocomposite Membranes for Water Desalination. ACS Nano, 2013, 7, 5308-5319.	7.3	331
8	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
9	Identification of Destabilized Metal Hydrides for Hydrogen Storage Using First Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 8769-8776.	1.2	273
10	Unusual Hydrogen Bonding in Water-Filled Carbon Nanotubes. Journal of the American Chemical Society, 2006, 128, 12090-12097.	6.6	261
11	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
12	Quantum Sieving in Carbon Nanotubes and Zeolites. Physical Review Letters, 1999, 82, 956-959.	2.9	247
13	Equation of State for Lennard-Jones Chains. The Journal of Physical Chemistry, 1994, 98, 6413-6419.	2.9	237
14	Optimization of Carbon Nanotube Arrays for Hydrogen Adsorption. Journal of Physical Chemistry B, 1999, 103, 4809-4813.	1.2	203
15	MATERIALS SCIENCE: Making High-Flux Membranes with Carbon Nanotubes. Science, 2006, 312, 1003-1004.	6.0	195
16	Simulation of Adsorption of DNA on Carbon Nanotubes. Journal of the American Chemical Society, 2007, 129, 10438-10445.	6.6	194
17	Reactive canonical Monte Carlo. Molecular Physics, 1994, 81, 717-733.	0.8	191
18	An accurate H2â€"H2 interaction potential from first principles. Journal of Chemical Physics, 2000, 112, 4465-4473.	1.2	188

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19	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
20	Adsorption and diffusion of carbon dioxide and nitrogen through single-walled carbon nanotube membranes. Journal of Chemical Physics, 2006, 124, 054708.	1.2	175
21	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
22	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
23	Reaction Mechanism of Monoethanolamine with CO₂ in Aqueous Solution from Molecular Modeling. Journal of Physical Chemistry A, 2010, 114, 11844-11852.	1.1	161
24	Gas Adsorption on Heterogeneous Single-Walled Carbon Nanotube Bundles. Physical Review Letters, 2003, 91, 015504.	2.9	149
25	Diffusivities of Ar and Ne in Carbon Nanotubes. Molecular Simulation, 2003, 29, 677-684.	0.9	146
26	Transport Diffusion of Gases Is Rapid in Flexible Carbon Nanotubes. Journal of Physical Chemistry B, 2006, 110, 1971-1975.	1.2	146
27	Molecular simulation of hydrogen adsorption in charged single-walled carbon nanotubes. Journal of Chemical Physics, 1999, 111, 9778-9783.	1.2	145
28	Design of Lewis Pair-Functionalized Metal Organic Frameworks for CO₂ Hydrogenation. ACS Catalysis, 2015, 5, 2921-2928.	5.5	137
29	Molecular-dynamics simulations of methane hydrate dissociation. Journal of Chemical Physics, 2005, 123, 244503.	1.2	136
30	Computer Simulations of Hydrogen Adsorption on Graphite Nanofibers. Journal of Physical Chemistry B, 1999, 103, 277-281.	1.2	135
31	Beyond Ordered Materials: Understanding Catalytic Sites on Amorphous Solids. ACS Catalysis, 2017, 7, 7543-7557.	5.5	134
32	Assessing nanoparticle size effects on metal hydride thermodynamics using the Wulff construction. Nanotechnology, 2009, 20, 204001.	1.3	127
33	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
34	Molecular simulation of xenon adsorption on single-walled carbon nanotubes. Journal of Chemical Physics, 2001, 114, 4180-4185.	1.2	122
35	Thermal Conductivity of Methane Hydrate from Experiment and Molecular Simulation. Journal of Physical Chemistry B, 2007, 111, 13194-13205.	1.2	119
36	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

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37	CO2â^'Fluorocarbon and CO2â^'Hydrocarbon Interactions from First-Principles Calculations. Journal of Physical Chemistry A, 1998, 102, 2231-2236.	1.1	107
38	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
39	Simulation of chemical reaction equilibria by the reaction ensemble Monte Carlo method: a reviewâ€. Molecular Simulation, 2008, 34, 119-146.	0.9	102
40	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
41	Light isotope separation in carbon nanotubes through quantum molecular sieving. Physical Review B, 2001, 63, .	1.1	100
42	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
43	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.	1.5	97
44	Phase Behavior of Oxygen-Containing Polymers in CO2. Macromolecules, 2007, 40, 1332-1341.	2.2	95
45	Trapped CO2in Carbon Nanotube Bundles. Journal of Physical Chemistry B, 2003, 107, 12930-12941.	1.2	94
46	Phase equilibria for associating Lennard-Jones fluids from theory and simulation. Molecular Physics, 1992, 77, 1033-1053.	0.8	93
47	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
48	Path integral grand canonical Monte Carlo. Journal of Chemical Physics, 1997, 107, 5108-5117.	1.2	92
49	Atomically detailed models of gas mixture diffusion through CuBTC membranes. Microporous and Mesoporous Materials, 2009, 125, 101-106.	2.2	90
50	Adsorption and Diffusion of Hydrogen in a New Metalâ^'Organic Framework Material:â€‰ [Zn(bdc)(ted)0.5]. Journal of Physical Chemistry C, 2008, 112, 2911-2917.	1.5	89
51	Accurate Amorphous Silica Surface Models from First-Principles Thermodynamics of Surface Dehydroxylation. Langmuir, 2014, 30, 5133-5141.	1.6	89
52	Chemical Activation of Single-Walled Carbon Nanotubes for Hydrogen Adsorption. Journal of Physical Chemistry B, 2003, 107, 3752-3760.	1.2	88
53	Oxygenated Hydrocarbon Ionic Surfactants Exhibit CO2Solubility. Journal of the American Chemical Society, 2005, 127, 11754-11762.	6.6	85
54	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

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55	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
56	Hydrogen adsorption on graphite and in carbon slit pores from path integral simulations. Molecular Physics, 1998, 95, 299-309.	0.8	81
57	Screening Lewis Pair Moieties for Catalytic Hydrogenation of CO₂ in Functionalized UiO-66. ACS Catalysis, 2015, 5, 6219-6229.	5.5	80
58	Hydrogen storage in carbon nanotubes and graphitic nanofibers. Journal of Alloys and Compounds, 2002, 330-332, 659-665.	2.8	77
59	Catalytic hydrogenation of CO₂ to methanol in a Lewis pair functionalized MOF. Catalysis Science and Technology, 2016, 6, 8392-8405.	2.1	75
60	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
61	Vibrational behavior of adsorbed CO2 on single-walled carbon nanotubes. Journal of Chemical Physics, 2004, 120, 5377-5386.	1.2	73
62	Atomic Charges Derived from Electrostatic Potentials for Molecular and Periodic Systems. Journal of Physical Chemistry A, 2010, 114, 10225-10233.	1.1	70
63	Design and Evaluation of Nonfluorous CO₂-Soluble Oligomers and Polymers. Journal of Physical Chemistry B, 2009, 113, 14971-14980.	1.2	69
64	Histogram reweighting and finite-size scaling study of the Lennardâ€“Jones fluids. Fluid Phase Equilibria, 2001, 187-188, 171-191.	1.4	68
65	Effect of confinement by porous materials on chemical reaction kinetics. Journal of Chemical Physics, 2002, 116, 2138-2148.	1.2	67
66	Testing the Accuracy of Correlations for Multicomponent Mass Transport of Adsorbed Gases in Metalâ€'Organic Frameworks: Diffusion of H₂/CH₄ Mixtures in CuBTC. Langmuir, 2008, 24, 8254-8261.	1.6	67
67	Optimization of Xe adsorption kinetics in single walled carbon nanotubes. Journal of Chemical Physics, 2001, 115, 6691-6698.	1.2	65
68	First-Principles Study of Experimental and Hypothetical Mg(BH₄)₂ Crystal Structures. Journal of Physical Chemistry C, 2008, 112, 4391-4395.	1.5	61
69	Phase equilibrium of quantum fluids from simulation: Hydrogen and neon. Fluid Phase Equilibria, 1997, 132, 93-116.	1.4	60
70	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
71	Aminosilicone Solvents for CO₂ Capture. ChemSusChem, 2010, 3, 919-930.	3.6	57
72	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

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73	An Effective Potential for Adsorption of Polar Molecules on Graphite. Molecular Simulation, 2005, 31, 1-10.	0.9	55
74	Solubility of CO2 in CO2-philic oligomers; COSMOtherm predictions and experimental results. Fluid Phase Equilibria, 2009, 287, 26-32.	1.4	55
75	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
76			

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91	Phase transitions of adsorbed fluids computed from multiple-histogram reweighting. Molecular Physics, 2002, 100, 2139-2150.	0.8	41
92	Development of a Transferable Reactive Force Field for Cobalt. Journal of Physical Chemistry A, 2010, 114, 5855-5861.	1.1	41
93	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
94	Axial Phase of Quantum Fluids in Nanotubes. Journal of Low Temperature Physics, 2000, 120, 337-359.	0.6	39
95	The importance of chargeâ€“quadrupole interactions for H2adsorption and diffusion in CuBTC. Molecular Simulation, 2009, 35, 60-69.	0.9	39
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.	1.5	37
97	Perturbation theory and computer simulations for linear and ring model polymers. Journal of Chemical Physics, 1996, 104, 1729-1742.	1.2	36
98	Structural and Electronic Properties of Pt₁₃ Nanoclusters on Amorphous Silica Supports. Journal of Physical Chemistry C, 2015, 119, 2503-2512.	1.5	34
99	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
100	Noble gases on metal surfaces: Insights on adsorption site preference. Physical Review B, 2011, 84, .	1.1	33
101	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
102	Formation of Odd-Numbered Clusters ofCO2Adsorbed on Nanotube Bundles. Physical Review Letters, 2005, 94, 125701.	2.9	31
103	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
104	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
105	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
106	First-Principles Characterization of Amorphous Phases of MB₁₂H₁₂, M = Mg, Ca. Journal of Physical Chemistry C, 2010, 114, 14601-14605.	1.5	29
107	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
108	C60sphase diagram: A full free-energy analysis. Physical Review B, 1997, 55, 2808-2817.	1.1	28

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109	Vacancy clusters as entry ports for cesium intercalation in graphite. Carbon, 2011, 49, 3937-3952.	5.4	28
110	Displacement ofCO2by Xe in single-walled carbon nanotube bundles. Physical Review B, 2004, 70, .	1.1	26
111	Stability analysis of doped materials for reversible hydrogen storage in destabilized metal hydrides. Physical Review B, 2007, 76, .	1.1	26
112	Density functional theory study of CO2 capture with transition metal oxides and hydroxides. Journal of Chemical Physics, 2012, 136, 064516.	1.2	26
113	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
114	Impact of Support Interactions for Single-Atom Molybdenum Catalysts on Amorphous Silica. Industrial & Engineering Chemistry Research, 2016, 55, 12350-12357.	1.8	24
115	Layering and orientational ordering of propane on graphite: An experimental and simulation study. Journal of Chemical Physics, 2002, 117, 7719-7731.	1.2	23
116	Modeling of Diffusion of Acetone in UiO-66. Journal of Physical Chemistry C, 2020, 124, 28469-28478.	1.5	23
117	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
118	First Principles Study of Adsorption and Dissociation of CO on W(111). Journal of Physical Chemistry B, 2006, 110, 1344-1349.	1.2	21
119	First-Principles Investigation of Adsorption and Dissociation of Hydrogen on Mg2Si Surfaces. Journal of Physical Chemistry C, 2007, 111, 6910-6916.	1.5	21
120	Reaction of the Basal Plane of Graphite with the Methyl Radical. Journal of Physical Chemistry Letters, 2012, 3, 1680-1683.	2.1	21
121	Facile Anhydrous Proton Transport on Hydroxyl Functionalized Graphane. Physical Review Letters, 2017, 118, 186101.	2.9	21
122	Toward Understanding the Kinetics of CO₂ Capture on Sodium Carbonate. ACS Applied Materials & Interfaces, 2019, 11, 9033-9041.	4.0	21
123	Wetting transitions of hydrogen and deuterium on the surface of alkali metals. Physical Review B, 2003, 68, .	1.1	20
124	Prediction of CH4/H2 Mixture Selectivity in Zn(tbip) from Computer Simulations. Journal of Low Temperature Physics, 2009, 157, 268-276.	0.6	20
125	Gas sorption properties of zwitterion-functionalized carbon nanotubes. Journal of Membrane Science, 2013, 429, 88-94.	4.1	20
126	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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127	Thermodynamic properties and vapor pressures of polar fluids from a four-parameter corresponding-states method. International Journal of Thermophysics, 1987, 8, 717-735.	1.0	19
128	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
129	Mechanism of Isobutylene Polymerization: Quantum Chemical Insight into AlCl₃/H₂O-Catalyzed Reactions. ACS Catalysis, 2018, 8, 8006-8013.	5.5	19
130	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
131	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
132	H₂/CO₂ separations in multicomponent metal-adeninate MOFs with multiple chemically distinct pore environments. Chemical Science, 2020, 11, 12807-12815.	3.7	18
133	Adsorption separation of heavier isotope gases in subnanometer carbon pores. Nature Communications, 2021, 12, 546.	5.8	18
134	Efficiently Trained Deep Learning Potential for Graphane. Journal of Physical Chemistry C, 2021, 125, 14874-14882.	1.5	18
135	Characterization of Bulk Structure in Zinc Orthotitanate: A Density Functional Theory and EXAFS Investigation. Journal of the American Ceramic Society, 2008, 91, 584-590.	1.9	17
136	Predicting catalyst-support interactions between metal nanoparticles and amorphous silica supports. Surface Science, 2016, 652, 278-285.	0.8	17
137	Quantum chemistry benchmarking of binding and selectivity for lanthanide extractants. International Journal of Quantum Chemistry, 2018, 118, e25516.	1.0	17
138	Reactive Canonical Monte Carlo. Advances in Chemical Physics, 2007, , 461-481.	0.3	16
139	Inter- and Intratube Self-Diffusion in n-Heptane Adsorbed on Carbon Nanotubes. Journal of Physical Chemistry C, 2007, 111, 4578-4584.	1.5	16
140	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
141	Methyl Radical Reactivity on the Basal Plane of Graphite. Journal of Physical Chemistry C, 2012, 116, 18347-18357.	1.5	16
142	Computer Simulation Studies of Adsorption of Simple Gases on Alkali Metal Surfaces. Journal of Low Temperature Physics, 1998, 110, 653-658.	0.6	15
143	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
144	A corresponding states principle for physisorption and deviations for quantum fluids. Molecular Physics, 2008, 106, 1579-1585.	0.8	14

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145	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
146	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
147	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
148	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
149	Unraveling Anhydrous Proton Conduction in Hydroxygraphane. Journal of Physical Chemistry Letters, 2019, 10, 518-523.	2.1	13
150	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
151	Screening the activity of Lewis pairs for hydrogenation of CO₂. Molecular Simulation, 2017, 43, 821-827.	0.9	12
152	Fundamental Insights into the Reactivity and Utilization of Open Metal Sites in Cu(I)-MFU-4l. Organometallics, 2019, 38, 3453-3459.	1.1	12
153	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
154	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
155	Surface tension of quantum fluids from molecular simulations. Journal of Chemical Physics, 2004, 120, 8707-8715.	1.2	11
156	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
157	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
158	Adsorbed Gases in Bundles of Carbon Nanotubes. , 2008, , 187-210.		10
159	Surface reactions of AsH3, H2Se, and H2S on the Zn2TiO4(010) surface. Surface Science, 2011, 605, 818-823.	0.8	10
160	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
161	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
162	Adsorption and Diffusion of Fluids in Defective Carbon Nanotubes: Insights from Molecular Simulations. Langmuir, 2017, 33, 11834-11844.	1.6	9

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163	Graphamine: Amine-Functionalized Graphane for Intrinsic Anhydrous Proton Conduction. Journal of Physical Chemistry C, 2019, 123, 1566-1571.	1.5	9
164	Molar excess volumes of liquid hydrogen and neon mixtures from path integral simulation. Journal of Chemical Physics, 1999, 111, 724-729.	1.2	8
165	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
166	Adsorption of Hydrogen in Graphitic Slit Pores. International Journal of Thermophysics, 1998, 19, 835-844.	1.0	7
167	A Combined Experimental and Computational Study on Selected Physical Properties of Aminosilicones. Industrial & Engineering Chemistry Research, 2014, 53, 1334-1341.	1.8	7
168	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
169	Prediction of vaporâ€”liquid equilibria in binary mixtures containing polar components from an extended leeâ€”kesler corresponding-states technique. Fluid Phase Equilibria, 1989, 44, 255-272.	1.4	6
170	Identifying UiOâ€67 Metalâ€Organic Framework Defects and Binding Sites through Ammonia Adsorption. ChemSusChem, 2022, 15, .	3.6	6
171	Vibron hopping and bond anharmonicity in hot dense hydrogen. Journal of Chemical Physics, 2009, 130, 054502.	1.2	5
172	One-dimensional adsorption and diffusion in Zn(tbip). Molecular Simulation, 2011, 37, 640-646.	0.9	5
173	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
174	Understanding and Improving the Kinetics of Bulk Carbonation on Sodium Carbonate. Journal of Physical Chemistry C, 2020, 124, 23106-23115.	1.5	5
175	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
176	Application of an extended Lee-Kesler corresponding-states technique to prediction of vapor-liquid equilibria in multicomponent mixtures containing polar components. International Journal of Thermophysics, 1989, 10, 479-492.	1.0	4
177	Direct observation of molecularly-aligned molecules in the second physisorbed layer-CO/Ag(110). Chemical Physics Letters, 2006, 418, 90-95.	1.2	4
178	Influence of Surface Reactions on Complex Hydride Reversibility. Journal of Physical Chemistry C, 2008, 112, 18270-18279.	1.5	4
179	Deliquescence of NaBH4 from Density Functional Theory and Experiments. Industrial & Engineering Chemistry Research, 2013, 52, 13849-13861.	1.8	4
180	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

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181	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
182	Density functional theory calculations of the surface structure of the inverse spinel zinc orthotitanate. Journal of Physics Condensed Matter, 2008, 20, 095001.	0.7	3
183	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
184	Effect of Chain Length on the Dipole Moment of Polyisobutylene Succinate Anhydride. Industrial & Engineering Chemistry Research, 2022, 61, 2359-2365.	1.8	3
185	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
186	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
187	Fermiâ€“LÃ¶wdin orbital self-interaction correction of adsorption energies on transition metal ions. Journal of Chemical Physics, 2022, 156, 134102.	1.2	2
188	Hydrogen Adsorption in Single-Walled Carbon Nanotubes. , 2008, , 369-401.		1
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