Dapeng Cao

List of Publications by Year
in descending order

306 papers	23,292 citations	9264 74 h-index	9861 141 g-index
314 all docs	314 docs citations	314 times ranked	23572 citing authors

#	Article	IF	Citations
1	Targeted Synthesis of a Porous Aromatic Framework with High Stability and Exceptionally High Surface Area. Angewandte Chemie - International Edition, 2009, 48, 9457-9460.	13.8	1,272
2	A universal principle for a rational design of single-atom electrocatalysts. Nature Catalysis, 2018, 1, 339-348.	34.4	1,214
3	ZIF-derived in situ nitrogen-doped porous carbons as efficient metal-free electrocatalysts for oxygen reduction reaction. Energy and Environmental Science, 2014, 7, 442-450.	30.8	719
4	Recent Progress in MOFâ€Derived, Heteroatomâ€Doped Porous Carbons as Highly Efficient Electrocatalysts for Oxygen Reduction Reaction in Fuel Cells. Advanced Functional Materials, 2018, 28, 1704537.	14.9	552
5	Nitrogen-doped graphene nanosheets as anode materials for lithium ion batteries: a first-principles study. Journal of Materials Chemistry, 2012, 22, 8911.	6.7	517
6	Unveiling the high-activity origin of single-atom iron catalysts for oxygen reduction reaction. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 6626-6631.	7.1	500
7	Highly Efficient Electrocatalysts for Oxygen Reduction Based on 2D Covalent Organic Polymers Complexed with Nonâ€precious Metals. Angewandte Chemie - International Edition, 2014, 53, 2433-2437.	13.8	417
8	A facile and versatile method for preparation of colored TiO₂ with enhanced solar-driven photocatalytic activity. Nanoscale, 2014, 6, 10216-10223.	5.6	382
9	Flexible polydimethylsiloxane/multi-walled carbon nanotubes membranous metacomposites with negative permittivity. Polymer, 2017, 125, 50-57.	3.8	379
10	Superior electromagnetic interference shielding 3D graphene nanoplatelets/reduced graphene oxide foam/epoxy nanocomposites with high thermal conductivity. Journal of Materials Chemistry C, 2019, 7, 2725-2733.	5.5	342
11	Porous covalentâ€“organic materials: synthesis, clean energy application and design. Journal of Materials Chemistry A, 2013, 1, 2691-2718.	10.3	329
12	An amino group functionalized metalâ€“organic framework as a luminescent probe for highly selective sensing of Fe3+ ions. Journal of Materials Chemistry A, 2014, 2, 7662.	10.3	312
13	Single-atom cobalt electrocatalysts for foldable solid-state Zn-air battery. Nano Energy, 2018, 50, 691-698.	16.0	303
14	Nanoparticle Dispersion and Aggregation in Polymer Nanocomposites: Insights from Molecular Dynamics Simulation. Langmuir, 2011, 27, 7926-7933.	3.5	295
15	Nitrogenâ€Doped Holey Graphitic Carbon from 2D Covalent Organic Polymers for Oxygen Reduction. Advanced Materials, 2014, 26, 3315-3320.	21.0	292
16	MXenes for polymer matrix electromagnetic interference shielding composites: A review. Composites Communications, 2021, 24, 100653.	6.3	291
17	Vertical CoP Nanoarray Wrapped by N,Pâ€Doped Carbon for Hydrogen Evolution Reaction in Both Acidic and Alkaline Conditions. Advanced Energy Materials, 2019, 9, 1803970.	19.5	284
18	Heavy metal ion removal of wastewater by zeolite-imidazolate frameworks. Separation and Purification Technology, 2018, 194, 462-469.	7.9	277

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19	Zeolitic imidazolate framework-derived nitrogen-doped porous carbons as high performance supercapacitor electrode materials. Carbon, 2015, 85, 51-59.	10.3	275
20	Zeolitic imidazolate framework-8 as a luminescent material for the sensing of metal ions and small molecules. Journal of Materials Chemistry, 2011, 21, 6649.	6.7	255
21	Metalâ€“Organic Frameworks with Incorporated Carbon Nanotubes: Improving Carbon Dioxide and Methane Storage Capacities by Lithium Doping. Angewandte Chemie - International Edition, 2011, 50, 491-494.	13.8	255
22	Lithiumâ€Doped 3D Covalent Organic Frameworks: Highâ€Capacity Hydrogen Storage Materials. Angewandte Chemie - International Edition, 2009, 48, 4730-4733.	13.8	244
23	Selective adsorption of carbon dioxide by carbonized porous aromatic framework (PAF). Energy and Environmental Science, 2012, 5, 8370.	30.8	234
24	Controllable etching of MoS2 basal planes for enhanced hydrogen evolution through the formation of active edge sites. Nano Energy, 2018, 49, 634-643.	16.0	220
25	Synthesis of Luminescent Covalentâ€“Organic Polymers for Detecting Nitroaromatic Explosives and Small Organic Molecules. Macromolecular Rapid Communications, 2012, 33, 1184-1190.	3.9	213
26	Polymerâ€based EMI shielding composites with 3D conductive networks: A miniâ€review. SusMat, 2021, 1, 413-431.	14.9	212
27	Doping of Alkali, Alkaline-Earth, and Transition Metals in Covalent-Organic Frameworks for Enhancing CO₂ Capture by First-Principles Calculations and Molecular Simulations. ACS Nano, 2010, 4, 4225-4237.	14.6	206
28	Singleâ€Atom Ru Doping Induced Phase Transition of MoS₂ and S Vacancy for Hydrogen Evolution Reaction. Small Methods, 2019, 3, 1900653.	8.6	206
29	Cu,N-codoped Hierarchical Porous Carbons as Electrocatalysts for Oxygen Reduction Reaction. ACS Applied Materials & Interfaces, 2016, 8, 21431-21439.	8.0	205
30	Systematic Tuning and Multifunctionalization of Covalent Organic Polymers for Enhanced Carbon Capture. Journal of the American Chemical Society, 2015, 137, 13301-13307.	13.7	202
31	Molecular Dynamics Study on Nanoparticle Diffusion in Polymer Melts:â€‰ A Test of the Stokesâ€“Einstein Law. Journal of Physical Chemistry C, 2008, 112, 6653-6661.	3.1	195
32	Well-defined two dimensional covalent organic polymers: rational design, controlled syntheses, and potential applications. Polymer Chemistry, 2015, 6, 1896-1911.	3.9	189
33	Biomass-derived FeNi alloy and nitrogen-codoped porous carbons as highly efficient oxygen reduction and evolution bifunctional electrocatalysts for rechargeable Zn-air battery. Energy Storage Materials, 2018, 12, 277-283.	18.0	176
34	ZIF-derived porous carbon: a promising supercapacitor electrode material. Journal of Materials Chemistry A, 2014, 2, 12873.	10.3	171
35	A Rigid Nested Metalâ€“Organic Framework Featuring a Thermoresponsive Gating Effect Dominated by Counterions. Angewandte Chemie - International Edition, 2016, 55, 15027-15030.	13.8	166
36	Optimization of Single-Walled Carbon Nanotube Arrays for Methane Storage at Room Temperature. Journal of Physical Chemistry B, 2003, 107, 13286-13292.	2.6	155

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37	Amino-Functionalized Luminescent Metalâ€“Organic Framework Test Paper for Rapid and Selective Sensing of SO₂ Gas and Its Derivatives by Luminescence Turn-On Effect. Analytical Chemistry, 2018, 90, 3608-3614.	6.5	146
38	CNT@Cu₃(BTC)₂ and Metalâ€“Organic Frameworks for Separation of CO₂/CH₄ Mixture. Journal of Physical Chemistry C, 2011, 115, 19864-19871.	3.1	144
39	Covalent-organic polymers for carbon dioxide capture. Journal of Materials Chemistry, 2012, 22, 22663.	6.7	143
40	ZIF-derived nitrogen-doped porous carbons as highly efficient adsorbents for removal of organic compounds from wastewater. Chemical Engineering Journal, 2017, 323, 502-511.	12.7	140
41	Porous organic polymers as a platform for sensing applications. Chemical Society Reviews, 2022, 51, 2031-2080.	38.1	140
42	Multiscale simulation and modelling of adsorptive processes for energy gas storage and carbon dioxide capture in porous coordination frameworks. Energy and Environmental Science, 2010, 3, 1469.	30.8	138
43	Improved Classical United-Atom Force Field for Imidazolium-Based Ionic Liquids: Tetrafluoroborate, Hexafluorophosphate, Methylsulfate, Trifluoromethylsulfonate, Acetate, Trifluoroacetate, and Bis(trifluoromethylsulfonyl)amide. Journal of Physical Chemistry B, 2011, 115, 10027-10040.	2.6	138
44	Co,N-codoped nanotube/graphene 1D/2D heterostructure for efficient oxygen reduction and hydrogen evolution reactions. Journal of Materials Chemistry A, 2018, 6, 3926-3932.	10.3	136
45	Highly sensitive and selective detection of 2,4,6-trinitrophenol using covalent-organic polymer luminescent probes. Journal of Materials Chemistry A, 2015, 3, 92-96.	10.3	132
46	Constructing interconnected spherical hollow conductive networks in silver platelets/reduced graphene oxide foam/epoxy nanocomposites for superior electromagnetic interference shielding effectiveness. Nanoscale, 2019, 11, 22590-22598.	5.6	130
47	Molecular Sizes and Antibacterial Performance Relationships of Flexible Ionic Liquid Derivatives. Journal of the American Chemical Society, 2020, 142, 20257-20269.	13.7	128
48	One-pot melamine derived nitrogen doped magnetic carbon nanoadsorbents with enhanced chromium removal. Carbon, 2016, 109, 640-649.	10.3	125
49	Metal-organic framework as luminescence turn-on sensor for selective detection of metal ions: Absorbance caused enhancement mechanism. Sensors and Actuators B: Chemical, 2018, 256, 839-845.	7.8	116
50	Adsorption and Diffusion of Shale Gas Reservoirs in Modeled Clay Minerals at Different Geological Depths. Energy & Fuels, 2014, 28, 7467-7473.	5.1	113
51	Silicon Nanotube as a Promising Candidate for Hydrogen Storage:â€‰ From the First Principle Calculations to Grand Canonical Monte Carlo Simulations. Journal of Physical Chemistry C, 2008, 112, 5598-5604.	3.1	104
52	Color tunable porous organic polymer luminescent probes for selective sensing of metal ions and nitroaromatic explosives. Journal of Materials Chemistry C, 2015, 3, 8490-8494.	5.5	103
53	Nitrogen-doped graphitic carbons with encapsulated CoNi bimetallic nanoparticles as bifunctional electrocatalysts for rechargeable Znâ€“Air batteries. Carbon, 2019, 144, 8-14.	10.3	101
54	High Uptakes of Methane in Li-Doped 3D Covalent Organic Frameworks. Langmuir, 2010, 26, 220-226.	3.5	99

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55	High-Capacity Hydrogen Storage in Porous Aromatic Frameworks with Diamond-like Structure. Journal of Physical Chemistry Letters, 2010, 1, 978-981.	4.6	98
56	Polymerâ€“nanoparticle interfacial behavior revisited: A molecular dynamics study. Physical Chemistry Chemical Physics, 2011, 13, 13058.	2.8	96
57	Adsorption of CO₂, CH₄, CO₂/N₂ and CO₂/CH₄ in novel activated carbon beads: Preparation, measurements and simulation. AIChE Journal, 2011, 57, 3042-3051.	3.6	96
58	Preparation and characterization of zinc sulfide nanoparticles under high-gravity environment. Materials Research Bulletin, 2004, 39, 185-194.	5.2	95
59	Postsynthetic Lithium Modification of Covalent-Organic Polymers for Enhancing Hydrogen and Carbon Dioxide Storage. Journal of Physical Chemistry C, 2012, 116, 5974-5980.	3.1	95
60	Covalent organic polymer supported palladium catalysts for CO oxidation. Chemical Communications, 2013, 49, 5633.	4.1	95
61	Molecular dynamics simulation for insight into microscopic mechanism of polymer reinforcement. Physical Chemistry Chemical Physics, 2011, 13, 518-529.	2.8	94
62	Metal (Pd, Pt)-decorated carbon nanotubes for CO and NO sensing. Sensors and Actuators B: Chemical, 2011, 159, 171-177.	7.8	87
63	Nanoparticle hardness controls the internalization pathway for drug delivery. Nanoscale, 2015, 7, 2758-2769.	5.6	86
64	A Novel Zrâ€MOF as Fluorescence Turnâ€On Probe for Realâ€Time Detecting H₂S Gas and Fingerprint Identification. Small, 2018, 14, e1703822.	10.0	86
65	Local Structure Evolution and its Connection to Thermodynamic and Transport Properties of 1-Butyl-3-methylimidazolium Tetrafluoroborate and Water Mixtures by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 3249-3263.	2.6	85
66	Molecular simulation of displacement of shale gas by carbon dioxide at different geological depths. Chemical Engineering Science, 2016, 156, 121-127.	3.8	85
67	Nitrogen and Fluorine-Codoped Porous Carbons as Efficient Metal-Free Electrocatalysts for Oxygen Reduction Reaction in Fuel Cells. ACS Applied Materials & Interfaces, 2017, 9, 32859-32867.	8.0	83
68	Facile preparation of high-capacity hydrogen storage metal-organic frameworks: A combination of microwave-assisted solvothermal synthesis and supercritical activation. Chemical Engineering Science, 2010, 65, 3140-3146.	3.8	81
69	Porous covalent organic polymers as luminescent probes for highly selective sensing of Fe3+ and chloroform: Functional group effects. Sensors and Actuators B: Chemical, 2016, 226, 273-278.	7.8	80
70	A Three-Dimensional sp² Carbon-Conjugated Covalent Organic Framework. Journal of the American Chemical Society, 2021, 143, 15562-15566.	13.7	80
71	Computer simulations for the adsorption and separation of CO2/CH4/H2/N2 gases by UMCM-1 and UMCM-2 metal organic frameworks. Journal of Materials Chemistry, 2011, 21, 11259.	6.7	79
72	Active Site Identification and Evaluation Criteria of In Situ Grown CoTe and NiTe Nanoarrays for Hydrogen Evolution and Oxygen Evolution Reactions. Small Methods, 2019, 3, 1900113.	8.6	78

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73	Computational screening of porous carbons, zeolites, and metal organic frameworks for desulfurization and decarburization of biogas, natural gas, and flue gas. AICHE Journal, 2013, 59, 2928-2942.	3.6	77
74	Density functional theory for semiflexible and cyclic polyatomic fluids. Journal of Chemical Physics, 2004, 121, 4210-4220.	3.0	76
75	Flameâ€Retardant Polypropylene/Multiwall Carbon Nanotube Nanocomposites: Effects of Surface Functionalization and Surfactant Molecular Weight. Macromolecular Chemistry and Physics, 2014, 215, 327-340.	2.2	75
76	Hydrogen Adsorption Storage on Single-Walled Carbon Nanotube Arrays by a Combination of Classical Potential and Density Functional Theory. Journal of Physical Chemistry B, 2003, 107, 4942-4950.	2.6	73
77	Self-Diffusion of Methane in Single-Walled Carbon Nanotubes at Sub- and Supercritical Conditions. Langmuir, 2004, 20, 3759-3765.	3.5	73
78	Functional Group Modification of Metalâ€“Organic Frameworks for CO₂ Capture. Journal of Physical Chemistry C, 2012, 116, 10573-10579.	3.1	73
79	Significantly enhanced energy density of magnetite/polypyrrole nanocomposite capacitors at high rates by low magnetic fields. Advanced Composites and Hybrid Materials, 2018, 1, 127-134.	21.1	73
80	Phosphorousâ€“Nitrogenâ€Codoped Carbon Materials Derived from Metalâ€“Organic Frameworks as Efficient Electrocatalysts for Oxygen Reduction Reactions. European Journal of Inorganic Chemistry, 2016, 2016, 2100-2105.	2.0	70
81	Paraffin/polyethylene/graphite composite phase change materials with enhanced thermal conductivity and leakage-proof. Advanced Composites and Hybrid Materials, 2021, 4, 543-551.	21.1	69
82	Design of the Alkali-Metal-Doped WO₃ as a Near-Infrared Shielding Material for Smart Window. Industrial & Engineering Chemistry Research, 2014, 53, 17981-17988.	3.7	68
83	Understanding the Mechanism of Photocatalysis Enhancements in the Graphene-like Semiconductor Sheet/TiO2 Composites. Journal of Physical Chemistry C, 2014, 118, 5954-5960.	3.1	65
84	Lithium doping on metal-organic frameworks for enhancing H2 Storage. International Journal of Hydrogen Energy, 2012, 37, 946-950.	7.1	64
85	Molecular Dynamics Simulation of Diffusion of Shale Oils in Montmorillonite. Journal of Physical Chemistry C, 2016, 120, 8986-8991.	3.1	64
86	Facile preparation of biomass-derived bifunctional electrocatalysts for oxygen reduction and evolution reactions. International Journal of Hydrogen Energy, 2018, 43, 8611-8622.	7.1	64
87	Timeâ^'Temperature and Timeâ^'Concentration Superposition of Nanofilled Elastomers: A Molecular Dynamics Study. Macromolecules, 2009, 42, 2831-2842.	4.8	63
88	Modeling the selectivity of activated carbons for efficient separation of hydrogen and carbon dioxide. Carbon, 2005, 43, 1364-1370.	10.3	62
89	Carbon Dioxide Capture by PAFs and an Efficient Strategy To Fast Screen Porous Materials for Gas Separation. Journal of Physical Chemistry C, 2013, 117, 8353-8364.	3.1	62
90	Kinetic Charging Inversion in Ionic Liquid Electric Double Layers. Journal of Physical Chemistry Letters, 2014, 5, 2195-2200.	4.6	62

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91	Hydrogen Production via Efficient Formic Acid Decomposition: Engineering the Surface Structure of Pd-Based Alloy Catalysts by Design. ACS Catalysis, 2019, 9, 781-790.	11.2	62
92	Biomass-derived nitrogen-doped porous carbons (NPC) and NPC/ polyaniline composites as high performance supercapacitor materials. Engineered Science, 2018, , .	2.3	62
93	Density-functional theory and Monte Carlo simulation for the surface structure and correlation functions of freely jointed Lennard-Jones polymeric fluids. Journal of Chemical Physics, 2005, 122, 174708.	3.0	61
94	Surface Forces between Telechelic Brushes Revisited:Â The Origin of a Weak Attraction. Langmuir, 2006, 22, 2712-2718.	3.5	60
95	Static, rheological and mechanical properties of polymer nanocomposites studied by computer modeling and simulation. Physical Chemistry Chemical Physics, 2009, 11, 11365.	2.8	60
96	Poly(vinylidene fluoride) derived fluorine-doped magnetic carbon nanoadsorbents for enhanced chromium removal. Carbon, 2017, 115, 503-514.	10.3	60
97	Improving Energy Conversion Efficiency of Dye-Sensitized Solar Cells by Modifying TiO₂ Photoanodes with Nitrogen-Reduced Graphene Oxide. ACS Sustainable Chemistry and Engineering, 2014, 2, 1234-1240.	6.7	59
98	A Fully Conjugated 3D Covalent Organic Framework Exhibiting Bandâ€like Transport with Ultrahigh Electron Mobility. Angewandte Chemie - International Edition, 2021, 60, 9321-9325.	13.8	59
99	Microstructure of Block Copolymers near Selective Surfaces:â€‰ Theoretical Predictions and Configurational-Bias Monte Carlo Simulation. Macromolecules, 2005, 38, 971-978.	4.8	58
100	Two-dimensional graphitic C₃N₅ materials: promising metal-free catalysts and CO₂ adsorbents. Journal of Materials Chemistry A, 2018, 6, 7168-7174.	10.3	58
101	Capture of Trace Sulfur Gases from Binary Mixtures by Single-Walled Carbon Nanotube Arrays: A Molecular Simulation Study. Environmental Science & Technology, 2011, 45, 4832-4838.	10.0	57
102	Effect of Li Doping on Diffusion and Separation of Hydrogen and Methane in Covalent Organic Frameworks. Journal of Physical Chemistry C, 2012, 116, 12591-12598.	3.1	57
103	Highly selective detection of picric acid from multicomponent mixtures of nitro explosives by using COP luminescent probe. Sensors and Actuators B: Chemical, 2017, 243, 753-760.	7.8	56
104	Nitrogen-doped graphene as an excellent candidate for selective gas sensing. Science China Chemistry, 2014, 57, 911-917.	8.2	55
105	Regioselective Functionalization of Stable BNâ€Modified Luminescent Tetraphenes for Highâ€Resolution Fingerprint Imaging. Angewandte Chemie - International Edition, 2019, 58, 10132-10137.	13.8	55
106	Computer simulation for storage of methane and capture of carbon dioxide in carbon nanoscrolls by expansion of interlayer spacing. Carbon, 2010, 48, 3760-3768.	10.3	54
107	Revisiting the Dispersion Mechanism of Grafted Nanoparticles in Polymer Matrix: A Detailed Molecular Dynamics Simulation. Langmuir, 2011, 27, 15213-15222.	3.5	54
108	Determination of pore size distribution and adsorption of methane and CCl4 on activated carbon by molecular simulation. Carbon, 2002, 40, 2359-2365.	10.3	52

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109	Hydrogen Storage in Mesoporous Coordination Frameworks: Experiment and Molecular Simulation. Journal of Physical Chemistry C, 2009, 113, 15106-15109.	3.1	52
110	Synthesis of Cu@Pd core-shell nanowires with enhanced activity and stability for formic acid oxidation. Electrochimica Acta, 2014, 143, 44-48.	5.2	52
111	Probing the Structural Transition Kinetics and Charge Compensation of the P2-Na_{0.78}Al_{0.05}Ni_{0.33}Mn_{0.60}O₂ Cathode for Sodium Ion Batteries. ACS Applied Materials & Interfaces, 2019, 11, 24122-24131.	8.0	51
112	Oriented construction Cu3P and Ni2P heterojunction to boost overall water splitting. Chemical Engineering Journal, 2022, 448, 137706.	12.7	51
113	Revisiting density functionals for the primitive model of electric double layers. Journal of Chemical Physics, 2014, 140, 044714.	3.0	50
114	Li-Doped and Nondoped Covalent Organic Borosilicate Framework for Hydrogen Storage. Journal of Physical Chemistry C, 2010, 114, 3108-3114.	3.1	49
115	Absorption competition quenching mechanism of porous covalent organic polymer as luminescent sensor for selective sensing Fe³⁺. ChemistrySelect, 2017, 2, 1041-1047.	1.5	49
116	Toughening of polypropylene-ethylene copolymer with nanosized CaCO3 and styrene-butadiene-styrene. Journal of Applied Polymer Science, 2004, 94, 796-802.	2.6	47
117	Molecular Simulation of Novel Carbonaceous Materials for Hydrogen Storage. Nano Letters, 2004, 4, 1489-1492.	9.1	47
118	The Role of Shape Complementarity in the Protein-Protein Interactions. Scientific Reports, 2013, 3, 3271.	3.3	47
119	Nitrogen-doped porous carbons with ultrahigh specific surface area as bifunctional materials for dye removal of wastewater and supercapacitors. Applied Surface Science, 2018, 456, 184-194.	6.1	47
120	Polyaniline-coated Ru/Ni(OH)2 nanosheets for hydrogen evolution reaction over a wide pH range. Journal of Catalysis, 2019, 375, 249-256.	6.2	47
121	Unlocking the potential of P3 structure for practical Sodium-ion batteries by fabricating zero strain framework for Na+ intercalation. Energy Storage Materials, 2021, 37, 354-362.	18.0	47
122	Ultra-small Ru nanoparticles embedded on Feâ€“Ni(OH)₂ nanosheets for efficient water splitting at a large current density with long-term stability of 680 hours. Journal of Materials Chemistry A, 2022, 10, 4817-4824.	10.3	46
123	Li12Si60H60 Fullerene Composite: A Promising Hydrogen Storage Medium. ACS Nano, 2009, 3, 3294-3300.	14.6	45
124	Time-dependent density functional theory for ion diffusion in electrochemical systems. Journal of Physics Condensed Matter, 2014, 26, 284102.	1.8	45
125	Effect of Tail Architecture on Self-Assembly of Amphiphiles for Polymeric Micelles. Langmuir, 2009, 25, 2749-2756.	3.5	44
126	Adsorption and separation of CH4/CO2/N2/H2/CO mixtures in hexagonally ordered carbon nanopipes CMK-5. Chemical Engineering Science, 2011, 66, 2266-2276.	3.8	44

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127	Screening donor groups of organic dyes for dye-sensitized solar cells. RSC Advances, 2015, 5, 22892-22898.	3.6	44
128	Porous organic polymer nanotubes as luminescent probe for highly selective and sensitive detection of Fe3+. Science China Chemistry, 2017, 60, 1090-1097.	8.2	44
129	Dual active site tandem catalysis of metal hydroxyl oxides and single atoms for boosting oxygen evolution reaction. Applied Catalysis B: Environmental, 2021, 297, 120451.	20.2	44
130	Designing a Thermo-switchable Channel for Nanofluidic Controllable Transportation. ACS Nano, 2011, 5, 1102-1108.	14.6	43
131	SiH/TiO2 and GeH/TiO2 Heterojunctions: Promising TiO2-based Photocatalysts under Visible Light. Scientific Reports, 2014, 4, 4810.	3.3	43
132	Atomically dispersed Fe-Cu dual-site catalysts synergistically boosting oxygen reduction for hydrogen fuel cells. Chemical Engineering Journal, 2022, 446, 137112.	12.7	43
133	Density functional theory for adsorption of colloids on the polymer-tethered surfaces: Effect of polymer chain architecture. Journal of Chemical Physics, 2009, 130, 164901.	3.0	42
134	Layering, condensation, and evaporation of short chains in narrow slit pores. Journal of Chemical Physics, 2005, 122, 224701.	3.0	41
135	Selective adsorption of olefinâ€“paraffin on diamond-like frameworks: diamondyne and PAF-302. Journal of Materials Chemistry A, 2013, 1, 9433.	10.3	41
136	Adsorption of carbon dioxide of 1-site and 3-site models in pillared clays: A Gibbs ensemble Monte Carlo simulation. Journal of Colloid and Interface Science, 2007, 310, 391-401.	9.4	40
137	Grand Canonical Monte Carlo Simulation for Determination of Optimum Parameters for Adsorption of Supercritical Methane in Pillared Layered Pores. Journal of Colloid and Interface Science, 2002, 254, 1-7.	9.4	39
138	A hybrid method for predicting the microstructure of polymers with complex architecture: Combination of single-chain simulation with density functional theory. Journal of Chemical Physics, 2006, 124, 164904.	3.0	39
139	Conformation of a Spherical Polyelectrolyte Brush in the Presence of Oppositely Charged Linear Polyelectrolytes. Macromolecules, 2008, 41, 5477-5484.	4.8	39
140	Molecular dynamics simulation of dispersion and aggregation kinetics of nanorods in polymer nanocomposites. Polymer, 2014, 55, 1273-1281.	3.8	39
141	Adsorption and selectivity of CH 4 /CO 2 in functional group rich organic shales. Journal of Natural Gas Science and Engineering, 2017, 39, 82-89.	4.4	39
142	Surface segregation of Agâ€“Cuâ€“Au trimetallic clusters. Nanotechnology, 2007, 18, 475702.	2.6	38
143	Existence of a Glassy Layer in the Polymerâ€‹<scp>N</scp>anosheet Interface: Evidence from Molecular Dynamics. Macromolecular Theory and Simulations, 2014, 23, 36-48.	1.4	38
144	Heterogeneity Characterization of Ordered Mesoporous Carbon Adsorbent CMK-1 for Methane and Hydrogen Storage: GCMC Simulation and Comparison with Experiment. Journal of Physical Chemistry C, 2008, 112, 13024-13036.	3.1	37

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145	Diffusion and Separation of H₂, CH₄, CO₂, and N₂ in Diamond-Like Frameworks. Journal of Physical Chemistry C, 2015, 119, 6324-6330.	3.1	37
146	Synthesis of thermosensitive micelles based on poly(N-isopropylacrylamide) and poly(l-alanine) for controlled release of adriamycin. Chemical Engineering Journal, 2010, 159, 257-263.	12.7	36
147	Rational Design of Dithienopicenocarbazole-Based Dyes and a Prediction of Their Energy-Conversion Efficiency Characteristics for Dye-Sensitized Solar Cells. ACS Applied Energy Materials, 2018, 1, 1435-1444.	5.1	36
148	Adsorption of sodium salt of poly(acrylic) acid (PAANa) on nano-sized CaCO3 and dispersion of nano-sized CaCO3 in water. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2004, 232, 163-168.	4.7	35
149	Luminescent porous organic polymer nanotubes for highly selective sensing of H₂S. Materials Chemistry Frontiers, 2017, 1, 2643-2650.	5.9	35
150	Novel Chemical Sensor for CO and NO: Silicon Nanotube. Journal of Physical Chemistry C, 2011, 115, 12015-12022.	3.1	34
151	A spontaneous penetration mechanism of patterned nanoparticles across a biomembrane. Soft Matter, 2014, 10, 6844.	2.7	34
152	Monte Carlo data of dilute solutions of large spheres in binary hard sphere mixtures. Molecular Physics, 2000, 98, 619-624.	1.7	33
153	Structural transition and melting of onion-ring Pdâ€“Pt bimetallic clusters. Chemical Physics Letters, 2008, 461, 71-76.	2.6	33
154	Density functional theory for predicting polymeric forces against surface fouling. Soft Matter, 2010, 6, 4631.	2.7	33
155	Understanding Photoelectrochemical Properties of Bâ€“N Codoped Anatase TiO₂ for Solar Energy Conversion. Journal of Physical Chemistry C, 2013, 117, 15911-15917.	3.1	33
156	Uniaxial deformation of nanorod filled polymer nanocomposites: a coarse-grained molecular dynamics simulation. Physical Chemistry Chemical Physics, 2014, 16, 16039.	2.8	33
157	ZIF-Derived Nitrogen-Doped Porous Carbons for Xe Adsorption and Separation. Scientific Reports, 2016, 6, 21295.	3.3	33
158	Sulfur, Nitrogen and Fluorine Tripleâ€Doped Metalâ€Free Carbon Electrocatalysts for the Oxygen Reduction Reaction. ChemElectroChem, 2019, 6, 741-747.	3.4	33
159	COMPUTATIONAL SIMULATION OF ELASTOMER NANOCOMPOSITES: CURRENT PROGRESS AND FUTURE CHALLENGES. Rubber Chemistry and Technology, 2012, 85, 450-481.	1.2	32
160	A porous diamond carbon framework: a new carbon allotrope with extremely high gas adsorption and mechanical properties. Journal of Materials Chemistry A, 2013, 1, 3851.	10.3	32
161	Physically Adsorbed Metal Ions in Porous Supports as Electrocatalysts for Oxygen Evolution Reaction. Advanced Functional Materials, 2020, 30, 1909889.	14.9	32
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