Kwang S Kim

List of Publications by Year
in descending order

580 papers	70,632 citations	1697 104 h-index	764 249 g-index
598 all docs	598 docs citations	598 times ranked	61628 citing authors

#	Article	IF	Citations
1	Large-scale pattern growth of graphene films for stretchable transparent electrodes. Nature, 2009, 457, 706-710.	13.7	9,624
2	Roll-to-roll production of 30-inch graphene films for transparent electrodes. Nature Nanotechnology, 2010, 5, 574-578.	15.6	7,294
3	Functionalization of Graphene: Covalent and Non-Covalent Approaches, Derivatives and Applications. Chemical Reviews, 2012, 112, 6156-6214.	23.0	3,531
4	Perovskite solar cells with atomically coherent interlayers on SnO2 electrodes. Nature, 2021, 598, 444-450.	13.7	2,065
5	Noncovalent Functionalization of Graphene and Graphene Oxide for Energy Materials, Biosensing, Catalytic, and Biomedical Applications. Chemical Reviews, 2016, 116, 5464-5519.	23.0	1,942
6	Water-Dispersible Magnetite-Reduced Graphene Oxide Composites for Arsenic Removal. ACS Nano, 2010, 4, 3979-3986.	7.3	1,835
7	Tuning the Graphene Work Function by Electric Field Effect. Nano Letters, 2009, 9, 3430-3434.	4.5	1,255
8	Molecular Clusters of Ï€-Systems:â€‰ Theoretical Studies of Structures, Spectra, and Origin of Interaction Energies. Chemical Reviews, 2000, 100, 4145-4186.	23.0	984
9	Zero-dimensional, one-dimensional, two-dimensional and three-dimensional nanostructured materials for advanced electrochemical energy devices. Progress in Materials Science, 2012, 57, 724-803.	16.0	892
10	Nickel-Based Electrocatalysts for Energy-Related Applications: Oxygen Reduction, Oxygen Evolution, and Hydrogen Evolution Reactions. ACS Catalysis, 2017, 7, 7196-7225.	5.5	857
11	Imidazolium receptors for the recognition of anions. Chemical Society Reviews, 2006, 35, 355.	18.7	766
12	Prediction of very large values of magnetoresistance in a graphene nanoribbon device. Nature Nanotechnology, 2008, 3, 408-412.	15.6	747
13	Ultrathin Single-Crystalline Silver Nanowire Arrays Formed in an Ambient Solution Phase. Science, 2001, 294, 348-351.	6.0	644
14	Enhanced Differentiation of Human Neural Stem Cells into Neurons on Graphene. Advanced Materials, 2011, 23, H263-7.	11.1	626
15	Understanding of Assembly Phenomena by Aromaticâˆ'Aromatic Interactions:Â Benzene Dimer and the Substituted Systems. Journal of Physical Chemistry A, 2007, 111, 3446-3457.	1.1	617
16	Highly selective adsorption of Hg2+ by a polypyrroleâ€"reduced graphene oxide composite. Chemical Communications, 2011, 47, 3942.	2.2	576
17	Unique Sandwich Stacking of Pyrene-Adenine-Pyrene for Selective and Ratiometric Fluorescent Sensing of ATP at Physiological pH. Journal of the American Chemical Society, 2009, 131, 15528-15533.	6.6	551
18	Multicomponent electrocatalyst with ultralow Pt loading and high hydrogen evolution activity. Nature Energy, 2018, 3, 773-782.	19.8	542

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19	Single Atoms and Clusters Based Nanomaterials for Hydrogen Evolution, Oxygen Evolution Reactions, and Full Water Splitting. Advanced Energy Materials, 2019, 9, 1900624.	10.2	538
20	Fast DNA sequencing with a graphene-based nanochannel device. Nature Nanotechnology, 2011, 6, 162-165.	15.6	517
21	Environmental applications using graphene composites: water remediation and gas adsorption. Nanoscale, 2013, 5, 3149.	2.8	472
22	Rhodamine-Based Hg2+-Selective Chemodosimeter in Aqueous Solution:Â Fluorescent OFFâˆ'ON. Organic Letters, 2007, 9, 907-910.	2.4	435
23	Engineered Carbon-Nanomaterial-Based Electrochemical Sensors for Biomolecules. ACS Nano, 2016, 10, 46-80.	7.3	433
24	Recent progress in the development of anode and cathode catalysts for direct methanol fuel cells. Nano Energy, 2013, 2, 553-578.	8.2	415
25	Reduced graphene oxide-based hydrogels for the efficient capture of dye pollutants from aqueous solutions. Carbon, 2013, 56, 173-182.	5.4	409
26	UV/Ozone-Oxidized Large-Scale Graphene Platform with Large Chemical Enhancement in Surface-Enhanced Raman Scattering. ACS Nano, 2011, 5, 9799-9806.	7.3	350
27	Near-field focusing and magnification through self-assembled nanoscale spherical lenses. Nature, 2009, 460, 498-501.	13.7	338
28	Enhanced Cr(vi) removal using iron nanoparticle decorated graphene. Nanoscale, 2011, 3, 3583.	2.8	337
29	Highly selective CO2 capture on N-doped carbon produced by chemical activation of polypyrrole functionalized graphene sheets. Chemical Communications, 2012, 48, 735-737.	2.2	328
30	Surface-Directed Molecular Assembly of Pentacene on Monolayer Graphene for High-Performance Organic Transistors. Journal of the American Chemical Society, 2011, 133, 4447-4454.	6.6	309
31	Structures, energies, vibrational spectra, and electronic properties of water monomer to decamer. Journal of Chemical Physics, 2000, 112, 9759-9772.	1.2	291
32	Structures, binding energies, and spectra of isoenergetic water hexamer clusters: Extensive ab initio studies. Journal of Chemical Physics, 1998, 109, 5886-5895.	1.2	290
33	Fluorescent GTP-Sensing in Aqueous Solution of Physiological pH. Journal of the American Chemical Society, 2004, 126, 8892-8893.	6.6	286
34	Geometrical and Electronic Structures of Gold, Silver, and Goldâˆ'Silver Binary Clusters:Â Origins of Ductility of Gold and Goldâˆ'Silver Alloy Formation. Journal of Physical Chemistry B, 2003, 107, 9994-10005.	1.2	283
35	Revisiting small clusters of water molecules. Chemical Physics Letters, 1986, 131, 451-456.	1.2	282
36	Tripodal Nitro-Imidazolium Receptor for Anion Binding Driven by (Câˆ'H)+-â€‰-â€‰-X-Hydrogen Bonds. Organic Letters, 2002, 4, 2897-2900.	2.4	273

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37	Theoretical Investigations of Anionâˆ’Ï€ Interactions:â€‰ The Role of Anions and the Nature of Ï€ Systems. Journal of Physical Chemistry A, 2004, 108, 1250-1258.	1.1	260
38	Grapheneâ€Encapsulated Nanoparticleâ€Based Biosensor for the Selective Detection of Cancer Biomarkers. Advanced Materials, 2011, 23, 2221-2225.	11.1	260
39	On Binding Forces between Aromatic Ring and Quaternary Ammonium Compound. Journal of the American Chemical Society, 1994, 116, 7399-7400.	6.6	256
40	Comprehensive Energy Analysis for Various Types of Ï€-Interaction. Journal of Chemical Theory and Computation, 2009, 5, 515-529.	2.3	253
41	Self-Assembled Arrays of Organic Nanotubes with Infinitely Long One-Dimensional H-Bond Chains. Journal of the American Chemical Society, 2001, 123, 10748-10749.	6.6	248
42	Work-Function Engineering of Graphene Electrodes by Self-Assembled Monolayers for High-Performance Organic Field-Effect Transistors. Journal of Physical Chemistry Letters, 2011, 2, 841-845.	2.1	237
43	A Calix[4]imidazolium[2]pyridine as an Anion Receptor. Angewandte Chemie - International Edition, 2005, 44, 2899-2903.	7.2	235
44	Grapheneâ€“SnO₂composites for highly efficient photocatalytic degradation of methylene blue under sunlight. Nanotechnology, 2012, 23, 355705.	1.3	233
45	Highly selective CO2 capture by S-doped microporous carbon materials. Carbon, 2014, 66, 320-326.	5.4	230
46	Ab initio studies of the water dimer using large basis sets: The structure and thermodynamic energies. Journal of Chemical Physics, 1992, 97, 6649-6662.	1.2	229
47	Singleâ€Gate Bandgap Opening of Bilayer Graphene by Dual Molecular Doping. Advanced Materials, 2012, 24, 407-411.	11.1	228
48	Cationâˆ’Ï€ Interactions:â€‰ A Theoretical Investigation of the Interaction of Metallic and Organic Cations with Alkenes, Arenes, and Heteroarenes. Journal of Physical Chemistry A, 2003, 107, 1228-1238.	1.1	226
49	Comparative ab initio study of the structures, energetics and spectra of X[sup âˆ’]â‹…(H[sub 2]O)[sub n=1â€“4] [X=F,â€ŠCl,â€ŠBr,â€ŠI] clusters. Journal of Chemical Physics, 2000, 113, 5259.	1.2	225
50	Highâ€Performance Hydrogen Evolution by Ru Single Atoms and Nitridedâ€Ru Nanoparticles Implanted on Nâ€Doped Graphitic Sheet. Advanced Energy Materials, 2019, 9, 1900931.	10.2	224
51	Selective-Area Fluorination of Graphene with Fluoropolymer and Laser Irradiation. Nano Letters, 2012, 12, 2374-2378.	4.5	222
52	Oneâ€Step Synthesis of CoSâ€Doped Î²â€Co(OH)₂@Amorphous MoS₂₊<i>_x</i> Hybrid Catalyst Grown on Nickel Foam for Highâ€Performance Electrochemical Overall Water Splitting. Advanced Functional Materials, 2016, 26, 7386-7393.	7.8	217
53	Graphene-nanoplatelets-supported NiFe-MOF: high-efficiency and ultra-stable oxygen electrodes for sustained alkaline anion exchange membrane water electrolysis. Energy and Environmental Science, 2020, 13, 3447-3458.	15.6	197
54	Olefinic vs Aromatic Ï€âˆ’H Interaction:Â A Theoretical Investigation of the Nature of Interaction of First-row Hydrides with Ethene and Benzene. Journal of the American Chemical Society, 2001, 123, 3323-3331.	6.6	193

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55	Substituent Effects on the Edge-to-Face Aromatic Interactions. Journal of the American Chemical Society, 2005, 127, 4530-4537.	6.6	190
56	Transparent Flexible Organic Transistors Based on Monolayer Graphene Electrodes on Plastic. Advanced Materials, 2011, 23, 1752-1756.	11.1	189
57	Multi-heteroatom-doped carbon from waste-yeast biomass for sustained water splitting. Nature Sustainability, 2020, 3, 556-563.	11.5	186
58	Mesoporous Silicon Hollow Nanocubes Derived from Metalâ€“Organic Framework Template for Advanced Lithium-Ion Battery Anode. ACS Nano, 2017, 11, 4808-4815.	7.3	181
59	Tuning metal single atoms embedded in N_xC_y moieties toward high-performance electrocatalysis. Energy and Environmental Science, 2021, 14, 3455-3468.	15.6	176
60	New Fluorescent Photoinduced Electron Transfer Chemosensor for the Recognition of H2PO4-. Organic Letters, 2003, 5, 2083-2086.	2.4	172
61	Highly Effective Fluorescent Sensor for H2PO4-. Journal of Organic Chemistry, 2004, 69, 581-583.	1.7	170
62	Stable platinum nanoclusters on genomic DNAâ€“graphene oxide with a high oxygen reduction reaction activity. Nature Communications, 2013, 4, 2221.	5.8	169
63	Chromium Porphyrin Arrays As Spintronic Devices. Journal of the American Chemical Society, 2011, 133, 9364-9369.	6.6	167
64	Structures, energetics, and spectra of aquaâ€sodium(I): Thermodynamic effects and nonadditive interactions. Journal of Chemical Physics, 1995, 102, 839-849.	1.2	166
65	Insights into the Structures, Energetics, and Vibrations of Monovalent Cationâˆ’(Water)1-6Clustersâ€. Journal of Physical Chemistry A, 2004, 108, 2949-2958.	1.1	158
66	Inductionâ€Driven Stabilization of the Anionâ€“Ï€ Interaction in Electronâ€Rich Aromatics as the Key to Fluoride Inclusion in Imidazoliumâ€Cage Receptors. Chemistry - A European Journal, 2011, 17, 1163-1170.	1.7	157
67	Iron-Oxide-Supported Nanocarbon in Lithium-Ion Batteries, Medical, Catalytic, and Environmental Applications. ACS Nano, 2014, 8, 7571-7612.	7.3	157
68	Tuning Molecular Orbitals in Molecular Electronics and Spintronics. Accounts of Chemical Research, 2010, 43, 111-120.	7.6	155
69	Simple and Scalable Mechanochemical Synthesis of Noble Metal Catalysts with Single Atoms toward Highly Efficient Hydrogen Evolution. Advanced Functional Materials, 2020, 30, 2000531.	7.8	153
70	Molecular Recognition of Fluoride Anion:â€‰ Benzene-Based Tripodal Imidazolium Receptor. Journal of Organic Chemistry, 2003, 68, 2467-2470.	1.7	151
71	Highly Stable CO₂/N₂ and CO₂/CH₄ Selectivity in Hyper-Cross-Linked Heterocyclic Porous Polymers. ACS Applied Materials & Interfaces, 2014, 6, 7325-7333.	4.0	151
72	Structures and energetics of the water heptamer: Comparison with the water hexamer and octamer. Journal of Chemical Physics, 1999, 110, 9128-9134.	1.2	149

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73	Complete basis set limit of <i>Ab initio</i> binding energies and geometrical parameters for various typical types of complexes. Journal of Computational Chemistry, 2008, 29, 1208-1221.	1.5	144
74	Ambipolar Memory Devices Based on Reduced Graphene Oxide and Nanoparticles. Advanced Materials, 2010, 22, 2045-2049.	11.1	143
75	What is the global minimum energy structure of the water hexamer? The importance of nonadditive interactions. Journal of Chemical Physics, 1994, 100, 4484-4486.	1.2	138
76	Control of Graphene Fieldâ€Effect Transistors by Interfacial Hydrophobic Selfâ€Assembled Monolayers. Advanced Materials, 2011, 23, 3460-3464.	11.1	138
77	Ionophores and receptors using cation-Â interactions: Collarenes. Proceedings of the National Academy of Sciences of the United States of America, 1998, 95, 12094-12099.	3.3	137
78	Eigen and Zundel Forms of Small Protonated Water Clusters:â€‰ Structures and Infrared Spectra. Journal of Physical Chemistry A, 2007, 111, 10692-10702.	1.1	137
79	Molecular architecture using novel types of non-covalent Ï€-interactions involving aromatic neutrals, aromatic cations and Ï€-anions. CrystEngComm, 2013, 15, 1285.	1.3	136
80	Machine learning-based high throughput screening for nitrogen fixation on boron-doped single atom catalysts. Journal of Materials Chemistry A, 2020, 8, 5209-5216.	5.2	136
81	Structures, Magnetic Properties, and Aromaticity of Cyclacenes. Angewandte Chemie - International Edition, 1999, 38, 2256-2258.	7.2	135
82	Structures, spectra, and electronic properties of halide-water pentamers and hexamers, Xâˆ'(H2O)5,6 (X=F,Cl,Br,I): Ab initio study. Journal of Chemical Physics, 2002, 116, 5509-5520.	1.2	135
83	Quasi-Continuous Growth of Ultralong Carbon Nanotube Arrays. Journal of the American Chemical Society, 2005, 127, 15336-15337.	6.6	131
84	The Nature of a Wet Electron. Physical Review Letters, 1996, 76, 956-959.	2.9	130
85	Charge transfer to solvent (CTTS) energies of small Xâˆ'(H2O)n=1â€"4 (X=F, Cl, Br, I) clusters: Ab initio study. Journal of Chemical Physics, 2000, 112, 101-105.	1.2	130
86	Electrochemical integration of amorphous NiFe (oxy)hydroxides on surface-activated carbon fibers for high-efficiency oxygen evolution in alkaline anion exchange membrane water electrolysis. Journal of Materials Chemistry A, 2021, 9, 14043-14051.	5.2	127
87	A theoretical investigation of the nature of the Ï€-H interaction in etheneâ€"H2O, benzeneâ€"H2O, and benzeneâ€"(H2O)2. Journal of Chemical Physics, 1999, 111, 5838-5850.	1.2	125
88	Highly efficient organic photocatalysts discovered via a computer-aided-design strategy for visible-light-driven atom transfer radical polymerization. Nature Catalysis, 2018, 1, 794-804.	16.1	124
89	Ruthenium Coreâ€"Shell Engineering with Nickel Single Atoms for Selective Oxygen Evolution via Nondestructive Mechanism. Advanced Energy Materials, 2021, 11, 2003448.	10.2	124
90	Structures, energetics, and spectra of fluorideâ€"water clusters Fâˆ'(H2O)n, n=1â€"6: Ab initio study. Journal of Chemical Physics, 1999, 110, 9116-9127.	1.2	122

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91	Radioactive iodine capture and storage from water using magnetite nanoparticles encapsulated in polypyrrole. Journal of Hazardous Materials, 2018, 344, 576-584.	6.5	120
92	Superb water splitting activity of the electrocatalyst Fe3Co(PO4)4 designed with computation aid. Nature Communications, 2019, 10, 5195.	5.8	120
93	Application of quantum chemistry to nanotechnology: electron and spin transport in molecular devices. Chemical Society Reviews, 2009, 38, 2319.	18.7	119
94	Dissociation chemistry of hydrogen halides in water. Journal of Chemical Physics, 2004, 120, 9524-9535.	1.2	117
95	Size Control of Semimetal Bismuth Nanoparticles and the UVâˆ’Visible and IR Absorption Spectra. Journal of Physical Chemistry B, 2005, 109, 7067-7072.	1.2	117
96	Highly Efficient Oxygen Reduction Reaction Activity of Graphitic Tube Encapsulating Nitrided Co<i>_x</i>Fe<i>_y</i> Alloy. Advanced Energy Materials, 2018, 8, 1801002.	10.2	117
97	Quantum mechanical probabilistic structure of the benzene-water complex. Chemical Physics Letters, 1997, 265, 497-502.	1.2	113
98	Simultaneous Transfer and Doping of CVD-Grown Graphene by Fluoropolymer for Transparent Conductive Films on Plastic. ACS Nano, 2012, 6, 1284-1290.	7.3	113
99	Structures and spectra of iodideâ€“water clusters I[sup âˆ’](H[sub 2]O)[sub n=1â€“6]: An ab initio study. Journal of Chemical Physics, 2001, 114, 4461.	1.2	111
100	Magic and Antimagic Protonated Water Clusters: Exotic Structures with Unusual Dynamic Effects. Angewandte Chemie - International Edition, 2006, 45, 3795-3800.	7.2	108
101	Controlling Ferromagnetic Easy Axis in a Layered<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Single Crystal. Physical Review Letters, 2013, 110, 247201.	2.9	108
102	Characterization of Weak NHâˆ’Ï€ Intermolecular Interactions of Ammonia with Various Substituted Ï€-Systems. Journal of the American Chemical Society, 2006, 128, 5416-5426.	6.6	107
103	Hydrogenâ€Release Mechanisms in Lithium Amidoboranes. Chemistry - A European Journal, 2009, 15, 5598-5604.	1.7	107
104	Assembling Phenomena of Calix[4]hydroquinone Nanotube Bundles by One-Dimensional Short Hydrogen Bonding and Displaced Ï€âˆ’Ï€ Stacking. Journal of the American Chemical Society, 2002, 124, 14268-14279.	6.6	106
105	Quinoxalineâˆ’Imidazolium Receptors for Unique Sensing of Pyrophosphate and Acetate by Charge Transfer. Organic Letters, 2007, 9, 485-488.	2.4	106
106	Interactions of CO₂with various functional molecules. Physical Chemistry Chemical Physics, 2015, 17, 10925-10933.	1.3	106
107	Ab initio study of the complexation of benzene with ammonium cations. Chemical Physics Letters, 1995, 232, 67-71.	1.2	104
108	Weakly correlated one-dimensional indium chains on Si(111). Physical Review B, 2001, 64, .	1.1	104

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109	First-Principles Modeling of Non-Covalent Interactions in Supramolecular Systems: The Role of Many-Body Effects. Journal of Chemical Theory and Computation, 2012, 8, 4317-4322.	2.3	104
110	Novel Structures for the Excess Electron State of the Water Hexamer and the Interaction Forces Governing the Structures. Physical Review Letters, 1997, 79, 2038-2041.	2.9	103
111	Structures, energetics, and spectra of electronâ€“water clusters, eâˆ’â€“(H2O)2â€“6 and eâˆ’â€“HOD(D2O)1â€“5. Journal of Chemical Physics, 2003, 119, 187-194.	1.2	103
112	Immiscible bi-metal single-atoms driven synthesis of electrocatalysts having superb mass-activity and durability. Applied Catalysis B: Environmental, 2020, 270, 118896.	10.8	102
113	Cationâˆ’Ï€âˆ’Anion Interaction:â€‰ A Theoretical Investigation of the Role of Induction Energies. Journal of Physical Chemistry A, 2007, 111, 7980-7986.	1.1	101
114	Fullerolâ€“Titania Chargeâ€Transferâ€Mediated Photocatalysis Working under Visible Light. Chemistry - A European Journal, 2009, 15, 10843-10850.	1.7	101
115	Gap Opening of Graphene by Dual FeCl₃-Acceptor and K-Donor Doping. Journal of Physical Chemistry Letters, 2011, 2, 2577-2581.	2.1	101
116	High-Affinity-Assisted Nanoscale Alloys as Remarkable Bifunctional Catalyst for Alcohol Oxidation and Oxygen Reduction Reactions. ACS Nano, 2017, 11, 7729-7735.	7.3	101
117	Aquaâ€“potassium(I) complexes: Ab initio study. Journal of Chemical Physics, 1999, 111, 3995-4004.	1.2	100
118	Enhanced resolution beyond the Abbe diffraction limit with wavelength-scale solid immersion lenses. Optics Letters, 2010, 35, 2007.	1.7	100
119	Catalytic role of enzymes: Short strong H-bond-induced partial proton shuttles and charge redistributions. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 6373-6378.	3.3	99
120	Machine Learning for Predicting the Band Gaps of ABX₃ Perovskites from Elemental Properties. Journal of Physical Chemistry C, 2020, 124, 8905-8918.	1.5	99
121	Role of Lewis Acid(AlCl3)âˆ’Aromatic Ring Interactions in Friedelâˆ’Craft's Reaction:Â An ab Initio Study. Journal of Physical Chemistry A, 1998, 102, 2253-2255.	1.1	96
122	Extremely stable graphene electrodes doped with macromolecular acid. Nature Communications, 2018, 9, 2037.	5.8	96
123	Selective Fluorescent Detection of RNA in Living Cells by Using Imidazolium-Based Cyclophane. Journal of the American Chemical Society, 2013, 135, 90-93.	6.6	95
124	Origin of the magic numbers of water clusters with an excess electron. Journal of Chemical Physics, 2005, 122, 044309.	1.2	94
125	Fluorescent imidazolium receptors for the recognition of pyrophosphate. Tetrahedron, 2006, 62, 6065-6072.	1.0	94
126	Anthracene derivatives bearing two urea groups as fluorescent receptors for anions. Tetrahedron, 2005, 61, 4545-4550.	1.0	93

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127	Calix[n]imidazolium as a new class of positively charged homo-calix compounds. Nature Communications, 2013, 4, 1797.	5.8	93
128	Is the Molecular Berry Phase an Artifact of the Born-Oppenheimer Approximation?. Physical Review Letters, 2014, 113, 263004.	2.9	93
129	Synthesis and Electrical Characterization of Magnetic Bilayer Graphene Intercalate. Nano Letters, 2011, 11, 860-865.	4.5	92
130	Fluorobenzeneâ‹¯water and difluorobenzeneâ‹¯water systems: An ab initio investigation. Journal of Chemical Physics, 1999, 110, 8501-8512.	1.2	91
131	Crystalline-amorphous interface of mesoporous Ni2PÂ@ÂFePOxHy for oxygen evolution at high current density in alkaline-anion-exchange-membrane water-electrolyzer. Applied Catalysis B: Environmental, 2022, 306, 121127.	10.8	90
132	Anthracene Derivatives Bearing Thiourea and Glucopyranosyl Groups for the Highly Selective Chiral Recognition of Amino Acids:â€‰ Opposite Chiral Selectivities from Similar Binding Units. Journal of Organic Chemistry, 2008, 73, 301-304.	1.7	89
133	Cyameluric Acid as Anion-Ï€ Type Receptor for ClO₄^{âˆ’} and NO₃^{âˆ’}: Ï€-Stacked and Edge-to-Face Structures. Journal of Chemical Theory and Computation, 2008, 4, 1401-1407.	2.3	89
134	Carbon nanotube, graphene, nanowire, and moleculeâ€based electron and spin transport phenomena using the nonequilibrium Green's function method at the level of first principles theory. Journal of Computational Chemistry, 2008, 29, 1073-1083.	1.5	88
135	Recent Advancement of pâ€•and dâ€Block Elements, Single Atoms, and Grapheneâ€Based Photoelectrochemical Electrodes for Water Splitting. Advanced Energy Materials, 2020, 10, 2000280.	10.2	88
136	Ab initio molecular dynamics of liquid water using embedded-fragment second-order many-body perturbation theory towards its accurate property prediction. Scientific Reports, 2015, 5, 14358.	1.6	87
137	Nature of One-Dimensional Short Hydrogen Bonding:â€‰ Bond Distances, Bond Energies, and Solvent Effects. Journal of the American Chemical Society, 2004, 126, 2186-2193.	6.6	86
138	Suppressed Î²-Hydride Elimination in Palladium-Catalyzed Cascade Cyclizationâˆ’Coupling Reactions:â€‰ An Efficient Synthesis of 3-Arylmethylpyrrolidines. Organic Letters, 2000, 2, 1213-1216.	2.4	85
139	Selective n-Type Doping of Graphene by Photo-patterned Gold Nanoparticles. ACS Nano, 2011, 5, 3639-3644.	7.3	85
140	Ab Initio Study of the Structures, Energetics, and Spectra of Aquazinc(II). The Journal of Physical Chemistry, 1996, 100, 14329-14338.	2.9	84
141	Ab initio studies of the water hexamer: near degenerate structures. Chemical Physics Letters, 1991, 176, 41-45.	1.2	83
142	Water dimer to pentamer with an excess electron: Ab initio study. Journal of Chemical Physics, 1999, 111, 10077-10087.	1.2	83
143	Ab initio study of hydrated sodium halides NaX(H2O)1â€“6 (X=F, Cl, Br, and I). Journal of Chemical Physics, 2006, 124, 024321.	1.2	82
144	Harmonic vibrational frequencies of the water monomer and dimer: Comparison of various levels of ab initio theory. Journal of Chemical Physics, 1995, 102, 310-317.	1.2	80

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145	Molecular Cluster Bowl To Enclose a Single Electron. Journal of the American Chemical Society, 1997, 119, 9329-9330.	6.6	80
146	Structures, energies, and vibrational spectra of water undecamer and dodecamer: An ab initio study. Journal of Chemical Physics, 2001, 114, 10749-10756.	1.2	80
147	Highly Selective and Stable Carbon Dioxide Uptake in Polyindole-Derived Microporous Carbon Materials. Environmental Science & Technology, 2013, 47, 5467-5473.	4.6	80
148	Structure-mechanism-based engineering of chemical regulators targeting distinct pathological factors in Alzheimerâ€™s disease. Nature Communications, 2016, 7, 13115.	5.8	80
149	Control of the Ï€ plasmon in a single layer graphene by charge doping. Applied Physics Letters, 2011, 99, .	1.5	79
150	Interconnected Pt-Nanodendrite/DNA/Reduced-Graphene-Oxide Hybrid Showing Remarkable Oxygen Reduction Activity and Stability. ACS Nano, 2013, 7, 9223-9231.	7.3	79
151	Versatile pâ€Type Chemical Doping to Achieve Ideal Flexible Graphene Electrodes. Angewandte Chemie - International Edition, 2016, 55, 6197-6201.	7.2	78
152	Accelerated Bone Regeneration by Two-Photon Photoactivated Carbon Nitride Nanosheets. ACS Nano, 2017, 11, 742-751.	7.3	78
153	Entropy-driven structures of the water octamer. Chemical Physics Letters, 1994, 219, 243-246.	1.2	77
154	Van der Waals Epitaxial Double Heterostructure: InAs/Singleâ€Layer Graphene/InAs. Advanced Materials, 2013, 25, 6847-6853.	11.1	77
155	Prediction of Reorganization Free Energies for Biological Electron Transfer: A Comparative Study of Ru-Modified Cytochromes and a 4-Helix Bundle Protein. Journal of the American Chemical Society, 2010, 132, 17032-17040.	6.6	76
156	Triazine-Based Microporous Polymers for Selective Adsorption of CO₂. Journal of Physical Chemistry C, 2015, 119, 5395-5402.	1.5	76
157	Structural, electronic, and magnetic properties of a ferromagnetic semiconductor: Co-dopedTiO2rutile. Physical Review B, 2003, 68, .	1.1	75
158	Reversible CO₂adsorption by an activated nitrogen doped graphene/polyaniline material. Nanotechnology, 2013, 24, 235703.	1.3	75
159	Novel Amphi-Ionophores. Journal of Physical Chemistry B, 1998, 102, 461-463.	1.2	74
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