

Kwang S Kim

List of Publications by Citations

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583
papers

59,759
citations

97
h-index

231
g-index

598
ext. papers

65,331
ext. citations

8.4
avg, IF

7.85
L-index

#	Paper	IF	Citations
583	Large-scale pattern growth of graphene films for stretchable transparent electrodes. <i>Nature</i> , 2009 , 457, 706-10	50.4	8675
582	Roll-to-roll production of 30-inch graphene films for transparent electrodes. <i>Nature Nanotechnology</i> , 2010 , 5, 574-8	28.7	6507
581	Functionalization of graphene: covalent and non-covalent approaches, derivatives and applications. <i>Chemical Reviews</i> , 2012 , 112, 6156-214	68.1	3041
580	Water-dispersible magnetite-reduced graphene oxide composites for arsenic removal. <i>ACS Nano</i> , 2010 , 4, 3979-86	16.7	1672
579	Noncovalent Functionalization of Graphene and Graphene Oxide for Energy Materials, Biosensing, Catalytic, and Biomedical Applications. <i>Chemical Reviews</i> , 2016 , 116, 5464-519	68.1	1546
578	Tuning the graphene work function by electric field effect. <i>Nano Letters</i> , 2009 , 9, 3430-4	11.5	1073
577	Molecular Clusters of pi-Systems: Theoretical Studies of Structures, Spectra, and Origin of Interaction Energies. <i>Chemical Reviews</i> , 2000 , 100, 4145-86	68.1	935
576	Imidazolium receptors for the recognition of anions. <i>Chemical Society Reviews</i> , 2006 , 35, 355-60	58.5	726
575	Zero-dimensional, one-dimensional, two-dimensional and three-dimensional nanostructured materials for advanced electrochemical energy devices. <i>Progress in Materials Science</i> , 2012 , 57, 724-803	42.2	704
574	Prediction of very large values of magnetoresistance in a graphene nanoribbon device. <i>Nature Nanotechnology</i> , 2008 , 3, 408-12	28.7	682
573	Ultrathin single-crystalline silver nanowire arrays formed in an ambient solution phase. <i>Science</i> , 2001 , 294, 348-51	33.3	599
572	Understanding of assembly phenomena by aromatic-aromatic interactions: benzene dimer and the substituted systems. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 3446-57	2.8	584
571	Nickel-Based Electrocatalysts for Energy-Related Applications: Oxygen Reduction, Oxygen Evolution, and Hydrogen Evolution Reactions. <i>ACS Catalysis</i> , 2017 , 7, 7196-7225	13.1	568
570	Enhanced differentiation of human neural stem cells into neurons on graphene. <i>Advanced Materials</i> , 2011 , 23, H263-7	24	542
569	Perovskite solar cells with atomically coherent interlayers on SnO electrodes. <i>Nature</i> , 2021 , 598, 444-450	50.4	530
568	Unique sandwich stacking of pyrene-adenine-pyrene for selective and ratiometric fluorescent sensing of ATP at physiological pH. <i>Journal of the American Chemical Society</i> , 2009 , 131, 15528-33	16.4	514
567	Highly selective adsorption of Hg ²⁺ by a polypyrrole-reduced graphene oxide composite. <i>Chemical Communications</i> , 2011 , 47, 3942-4	5.8	509

566	Fast DNA sequencing with a graphene-based nanochannel device. <i>Nature Nanotechnology</i> , 2011 , 6, 162-58.7	46.2	462
565	Rhodamine-based Hg ²⁺ -selective chemodosimeter in aqueous solution: fluorescent OFF-ON. <i>Organic Letters</i> , 2007 , 9, 907-10	6.2	413
564	Environmental applications using graphene composites: water remediation and gas adsorption. <i>Nanoscale</i> , 2013 , 5, 3149-71	7.7	407
563	Reduced graphene oxide-based hydrogels for the efficient capture of dye pollutants from aqueous solutions. <i>Carbon</i> , 2013 , 56, 173-182	10.4	349
562	Recent progress in the development of anode and cathode catalysts for direct methanol fuel cells. <i>Nano Energy</i> , 2013 , 2, 553-578	17.1	348
561	Engineered Carbon-Nanomaterial-Based Electrochemical Sensors for Biomolecules. <i>ACS Nano</i> , 2016 , 10, 46-80	16.7	337
560	Multicomponent electrocatalyst with ultralow Pt loading and high hydrogen evolution activity. <i>Nature Energy</i> , 2018 , 3, 773-782	62.3	330
559	Enhanced Cr(vi) removal using iron nanoparticle decorated graphene. <i>Nanoscale</i> , 2011 , 3, 3583-5	7.7	310
558	UV/ozone-oxidized large-scale graphene platform with large chemical enhancement in surface-enhanced Raman scattering. <i>ACS Nano</i> , 2011 , 5, 9799-806	16.7	298
557	Highly selective CO ₂ capture on N-doped carbon produced by chemical activation of polypyrrole functionalized graphene sheets. <i>Chemical Communications</i> , 2012 , 48, 735-7	5.8	297
556	Single Atoms and Clusters Based Nanomaterials for Hydrogen Evolution, Oxygen Evolution Reactions, and Full Water Splitting. <i>Advanced Energy Materials</i> , 2019 , 9, 1900624	21.8	294
555	Near-field focusing and magnification through self-assembled nanoscale spherical lenses. <i>Nature</i> , 2009 , 460, 498-501	50.4	290
554	Surface-directed molecular assembly of pentacene on monolayer graphene for high-performance organic transistors. <i>Journal of the American Chemical Society</i> , 2011 , 133, 4447-54	16.4	287
553	Structures, binding energies, and spectra of isoenergetic water hexamer clusters: Extensive ab initio studies. <i>Journal of Chemical Physics</i> , 1998 , 109, 5886-5895	3.9	280
552	Geometrical and Electronic Structures of Gold, Silver, and GoldSilver Binary Clusters: Origins of Ductility of Gold and GoldSilver Alloy Formation. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 9994-10005	3.4	275
551	Fluorescent GTP-sensing in aqueous solution of physiological pH. <i>Journal of the American Chemical Society</i> , 2004 , 126, 8892-3	16.4	274
550	Structures, energies, vibrational spectra, and electronic properties of water monomer to decamer. <i>Journal of Chemical Physics</i> , 2000 , 112, 9759-9772	3.9	270
549	Revisiting small clusters of water molecules. <i>Chemical Physics Letters</i> , 1986 , 131, 451-456	2.5	269

548	Tripodal nitro-imidazolium receptor for anion binding driven by (C-H) \cdots X- hydrogen bonds. <i>Organic Letters</i> , 2002 , 4, 2897-900	6.2	257
547	Theoretical Investigations of Anion- π Interactions: The Role of Anions and the Nature of π Systems. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 1250-1258	2.8	248
546	Graphene-encapsulated nanoparticle-based biosensor for the selective detection of cancer biomarkers. <i>Advanced Materials</i> , 2011 , 23, 2221-5	24	238
545	Comprehensive Energy Analysis for Various Types of π Interaction. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 515-29	6.4	235
544	On Binding Forces between Aromatic Ring and Quaternary Ammonium Compound. <i>Journal of the American Chemical Society</i> , 1994 , 116, 7399-7400	16.4	235
543	Self-assembled arrays of organic nanotubes with infinitely long one-dimensional H-bond chains. <i>Journal of the American Chemical Society</i> , 2001 , 123, 10748-9	16.4	233
542	A calix[4]imidazolium[2]pyridine as an anion receptor. <i>Angewandte Chemie - International Edition</i> , 2005 , 44, 2899-903	16.4	226
541	Work-Function Engineering of Graphene Electrodes by Self-Assembled Monolayers for High-Performance Organic Field-Effect Transistors. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 841-5	6.4	224
540	Comparative ab initio study of the structures, energetics and spectra of X $_n$ (H $_2$ O) $_n$ =1 $_n$ [X=F, Cl, Br, I] clusters. <i>Journal of Chemical Physics</i> , 2000 , 113, 5259	3.9	213
539	Single-gate bandgap opening of bilayer graphene by dual molecular doping. <i>Advanced Materials</i> , 2012 , 24, 407-11	24	212
538	Cation- π Interactions: A Theoretical Investigation of the Interaction of Metallic and Organic Cations with Alkenes, Arenes, and Heteroarenes. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 1228-1238	2.8	212
537	Ab initio studies of the water dimer using large basis sets: The structure and thermodynamic energies. <i>Journal of Chemical Physics</i> , 1992 , 97, 6649-6662	3.9	211
536	Graphene-SnO $_2$ composites for highly efficient photocatalytic degradation of methylene blue under sunlight. <i>Nanotechnology</i> , 2012 , 23, 355705	3.4	208
535	Selective-area fluorination of graphene with fluoropolymer and laser irradiation. <i>Nano Letters</i> , 2012 , 12, 2374-8	11.5	201
534	Olefinic vs. aromatic π -H interaction: a theoretical investigation of the nature of interaction of first-row hydrides with ethene and benzene. <i>Journal of the American Chemical Society</i> , 2001 , 123, 3323-31	16.4	183
533	Substituent effects on the edge-to-face aromatic interactions. <i>Journal of the American Chemical Society</i> , 2005 , 127, 4530-7	16.4	182
532	Highly selective CO $_2$ capture by S-doped microporous carbon materials. <i>Carbon</i> , 2014 , 66, 320-326	10.4	178
531	Transparent flexible organic transistors based on monolayer graphene electrodes on plastic. <i>Advanced Materials</i> , 2011 , 23, 1752-6	24	175

530	Highly effective fluorescent sensor for H ₂ PO ₄ (-). <i>Journal of Organic Chemistry</i> , 2004 , 69, 581-3	4.2	169
529	New fluorescent photoinduced electron transfer chemosensor for the recognition of H ₂ PO ₄ -. <i>Organic Letters</i> , 2003 , 5, 2083-6	6.2	166
528	One-Step Synthesis of CoS-Doped [Co(OH) ₂ @Amorphous MoS ₂ +x Hybrid Catalyst Grown on Nickel Foam for High-Performance Electrochemical Overall Water Splitting. <i>Advanced Functional Materials</i> , 2016 , 26, 7386-7393	15.6	166
527	Structures, energetics, and spectra of aqua-sodium(I): Thermodynamic effects and nonadditive interactions. <i>Journal of Chemical Physics</i> , 1995 , 102, 839-849	3.9	157
526	Stable platinum nanoclusters on genomic DNA-graphene oxide with a high oxygen reduction reaction activity. <i>Nature Communications</i> , 2013 , 4, 2221	17.4	156
525	Chromium porphyrin arrays as spintronic devices. <i>Journal of the American Chemical Society</i> , 2011 , 133, 9364-9	16.4	149
524	Insights into the Structures, Energetics, and Vibrations of Monovalent Cation(Water) ₁₋₆ Clusters. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 2949-2958	2.8	148
523	Tuning molecular orbitals in molecular electronics and spintronics. <i>Accounts of Chemical Research</i> , 2010 , 43, 111-20	24.3	147
522	Structures and energetics of the water heptamer: Comparison with the water hexamer and octamer. <i>Journal of Chemical Physics</i> , 1999 , 110, 9128-9134	3.9	145
521	Induction-driven stabilization of the anion-π interaction in electron-rich aromatics as the key to fluoride inclusion in imidazolium-cage receptors. <i>Chemistry - A European Journal</i> , 2011 , 17, 1163-70	4.8	144
520	Molecular recognition of fluoride anion: benzene-based tripodal imidazolium receptor. <i>Journal of Organic Chemistry</i> , 2003 , 68, 2467-70	4.2	143
519	Complete basis set limit of Ab initio binding energies and geometrical parameters for various typical types of complexes. <i>Journal of Computational Chemistry</i> , 2008 , 29, 1208-21	3.5	142
518	Mesoporous Silicon Hollow Nanocubes Derived from Metal-Organic Framework Template for Advanced Lithium-Ion Battery Anode. <i>ACS Nano</i> , 2017 , 11, 4808-4815	16.7	141
517	Ambipolar memory devices based on reduced graphene oxide and nanoparticles. <i>Advanced Materials</i> , 2010 , 22, 2045-9	24	138
516	Ionophores and receptors using cation-π interactions: collarenes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1998 , 95, 12094-9	11.5	133
515	What is the global minimum energy structure of the water hexamer? The importance of nonadditive interactions. <i>Journal of Chemical Physics</i> , 1994 , 100, 4484-4486	3.9	133
514	High-Performance Hydrogen Evolution by Ru Single Atoms and Nitrided-Ru Nanoparticles Implanted on N-Doped Graphitic Sheet. <i>Advanced Energy Materials</i> , 2019 , 9, 1900931	21.8	131
513	Highly stable CO ₂ /N ₂ and CO ₂ /CH ₄ selectivity in hyper-cross-linked heterocyclic porous polymers. <i>ACS Applied Materials & Interfaces</i> , 2014 , 6, 7325-33	9.5	131

512	Structures, spectra, and electronic properties of halide-water pentamers and hexamers, $X(H_2O)_5,6$ (X=F,Cl,Br,I): Ab initio study. <i>Journal of Chemical Physics</i> , 2002 , 116, 5509-5520	3.9	131
511	Iron-oxide-supported nanocarbon in lithium-ion batteries, medical, catalytic, and environmental applications. <i>ACS Nano</i> , 2014 , 8, 7571-612	16.7	128
510	Structures, Magnetic Properties, and Aromaticity of Cyclacenes. <i>Angewandte Chemie - International Edition</i> , 1999 , 38, 2256-2258	16.4	126
509	Charge transfer to solvent (CTTS) energies of small $X(H_2O)_n=1-8$ (X=F, Cl, Br, I) clusters: Ab initio study. <i>Journal of Chemical Physics</i> , 2000 , 112, 101-105	3.9	125
508	Eigen and Zundel forms of small protonated water clusters: structures and infrared spectra. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 10692-702	2.8	123
507	A theoretical investigation of the nature of the π -H interaction in ethene π H ₂ O, benzene π H ₂ O, and benzene π (H ₂ O) ₂ . <i>Journal of Chemical Physics</i> , 1999 , 111, 5838-5850	3.9	123
506	Quasi-continuous growth of ultralong carbon nanotube arrays. <i>Journal of the American Chemical Society</i> , 2005 , 127, 15336-7	16.4	122
505	The nature of a wet electron. <i>Physical Review Letters</i> , 1996 , 76, 956-959	7.4	121
504	Control of graphene field-effect transistors by interfacial hydrophobic self-assembled monolayers. <i>Advanced Materials</i> , 2011 , 23, 3460-4	24	119
503	Molecular architecture using novel types of non-covalent π -interactions involving aromatic neutrals, aromatic cations and π -anions. <i>CrystEngComm</i> , 2013 , 15, 1285	3.3	117
502	Structures, energetics, and spectra of fluoride-water clusters $F(H_2O)_n$, $n=1-8$: Ab initio study. <i>Journal of Chemical Physics</i> , 1999 , 110, 9116-9127	3.9	115
501	Dissociation chemistry of hydrogen halides in water. <i>Journal of Chemical Physics</i> , 2004 , 120, 9524-35	3.9	111
500	Application of quantum chemistry to nanotechnology: electron and spin transport in molecular devices. <i>Chemical Society Reviews</i> , 2009 , 38, 2319-33	58.5	109
499	Quantum mechanical probabilistic structure of the benzene-water complex. <i>Chemical Physics Letters</i> , 1997 , 265, 497-502	2.5	108
498	Magic and antimagic protonated water clusters: exotic structures with unusual dynamic effects. <i>Angewandte Chemie - International Edition</i> , 2006 , 45, 3795-800	16.4	106
497	Hydrogen-release mechanisms in lithium amidoboranes. <i>Chemistry - A European Journal</i> , 2009 , 15, 5598-603	4.8	105
496	Size control of semimetal bismuth nanoparticles and the UV-visible and IR absorption spectra. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 7067-72	3.4	104
495	Characterization of weak NH- π intermolecular interactions of ammonia with various substituted π -systems. <i>Journal of the American Chemical Society</i> , 2006 , 128, 5416-26	16.4	104

494	Simultaneous transfer and doping of CVD-grown graphene by fluoropolymer for transparent conductive films on plastic. <i>ACS Nano</i> , 2012 , 6, 1284-90	16.7	103
493	Structures and spectra of iodide-water clusters $I[H_2O]_n$: An ab initio study. <i>Journal of Chemical Physics</i> , 2001 , 114, 4461	3.9	103
492	Weakly correlated one-dimensional indium chains on Si(111). <i>Physical Review B</i> , 2001 , 64,	3.3	101
491	Assembling phenomena of calix[4]hydroquinone nanotube bundles by one-dimensional short hydrogen bonding and displaced pi-pi stacking. <i>Journal of the American Chemical Society</i> , 2002 , 124, 14268-79	16.4	101
490	Quinoxaline-imidazolium receptors for unique sensing of pyrophosphate and acetate by charge transfer. <i>Organic Letters</i> , 2007 , 9, 485-8	6.2	100
489	First-Principles Modeling of Non-Covalent Interactions in Supramolecular Systems: The Role of Many-Body Effects. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 4317-22	6.4	98
488	Structures, energetics, and spectra of electron-water clusters, $e(H_2O)_2$ and $eHOD(D_2O)_1$. <i>Journal of Chemical Physics</i> , 2003 , 119, 187-194	3.9	98
487	Ab initio study of the complexation of benzene with ammonium cations. <i>Chemical Physics Letters</i> , 1995 , 232, 67-71	2.5	98
486	Aqua-potassium(I) complexes: Ab initio study. <i>Journal of Chemical Physics</i> , 1999 , 111, 3995-4004	3.9	96
485	Gap Opening of Graphene by Dual $FeCl_3$ -Acceptor and K-Donor Doping. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 2577-2581	6.4	95
484	Cation-pi-anion interaction: a theoretical investigation of the role of induction energies. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 7980-6	2.8	94
483	Controlling ferromagnetic easy axis in a layered MoS_2 single crystal. <i>Physical Review Letters</i> , 2013 , 110, 247201	7.4	93
482	Novel Structures for the Excess Electron State of the Water Hexamer and the Interaction Forces Governing the Structures. <i>Physical Review Letters</i> , 1997 , 79, 2038-2041	7.4	93
481	Fluorescent imidazolium receptors for the recognition of pyrophosphate. <i>Tetrahedron</i> , 2006 , 62, 6065-6072	7.2	91
480	Anthracene derivatives bearing two urea groups as fluorescent receptors for anions. <i>Tetrahedron</i> , 2005 , 61, 4545-4550	2.4	91
479	Origin of the magic numbers of water clusters with an excess electron. <i>Journal of Chemical Physics</i> , 2005 , 122, 44309	3.9	91
478	Catalytic role of enzymes: short strong H-bond-induced partial proton shuttles and charge redistributions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2000 , 97, 6373-8	11.5	91
477	Fullerol-titania charge-transfer-mediated photocatalysis working under visible light. <i>Chemistry - A European Journal</i> , 2009 , 15, 10843-50	4.8	90

476	Highly Efficient Oxygen Reduction Reaction Activity of Graphitic Tube Encapsulating Nitrided CoxFey Alloy. <i>Advanced Energy Materials</i> , 2018 , 8, 1801002	21.8	90
475	Fluorobenzene?water and difluorobenzene?water systems: An ab initio investigation. <i>Journal of Chemical Physics</i> , 1999 , 110, 8501-8512	3.9	89
474	Calix[n]imidazolium as a new class of positively charged homo-calix compounds. <i>Nature Communications</i> , 2013 , 4, 1797	17.4	88
473	Role of Lewis Acid(AlCl3)Aromatic Ring Interactions in FriedelCraft's Reaction: An ab Initio Study. <i>Journal of Physical Chemistry A</i> , 1998 , 102, 2253-2255	2.8	88
472	Selective fluorescent detection of RNA in living cells by using imidazolium-based cyclophane. <i>Journal of the American Chemical Society</i> , 2013 , 135, 90-3	16.4	87
471	Anthracene derivatives bearing thiourea and glucopyranosyl groups for the highly selective chiral recognition of amino acids: opposite chiral selectivities from similar binding units. <i>Journal of Organic Chemistry</i> , 2008 , 73, 301-4	4.2	85
470	Synthesis and electrical characterization of magnetic bilayer graphene intercalate. <i>Nano Letters</i> , 2011 , 11, 860-5	11.5	83
469	Enhanced resolution beyond the Abbe diffraction limit with wavelength-scale solid immersion lenses. <i>Optics Letters</i> , 2010 , 35, 2007-9	3	82
468	Interactions of CO2 with various functional molecules. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 10925-33	3.6	81
467	Is the molecular Berry phase an artifact of the Born-Oppenheimer approximation?. <i>Physical Review Letters</i> , 2014 , 113, 263004	7.4	81
466	Cyamelic Acid as Anion-Type Receptor for ClO4(-) and NO3(-): Stacked and Edge-to-Face Structures. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 1401-7	6.4	81
465	High-Affinity-Assisted Nanoscale Alloys as Remarkable Bifunctional Catalyst for Alcohol Oxidation and Oxygen Reduction Reactions. <i>ACS Nano</i> , 2017 , 11, 7729-7735	16.7	79
464	Carbon nanotube, graphene, nanowire, and molecule-based electron and spin transport phenomena using the nonequilibrium Green's function method at the level of first principles theory. <i>Journal of Computational Chemistry</i> , 2008 , 29, 1073-83	3.5	79
463	Water dimer to pentamer with an excess electron: Ab initio study. <i>Journal of Chemical Physics</i> , 1999 , 111, 10077-10087	3.9	78
462	Ab initio studies of the water hexamer: near degenerate structures. <i>Chemical Physics Letters</i> , 1991 , 176, 41-45	2.5	78
461	Highly efficient organic photocatalysts discovered via a computer-aided-design strategy for visible-light-driven atom transfer radical polymerization. <i>Nature Catalysis</i> , 2018 , 1, 794-804	36.5	78
460	Multi-heteroatom-doped carbon from waste-yeast biomass for sustained water splitting. <i>Nature Sustainability</i> , 2020 , 3, 556-563	22.1	77
459	Selective n-type doping of graphene by photo-patterned gold nanoparticles. <i>ACS Nano</i> , 2011 , 5, 3639-44	16.7	77

458	Molecular Cluster Bowl To Enclose a Single Electron. <i>Journal of the American Chemical Society</i> , 1997 , 119, 9329-9330	16.4	76
457	Ab initio study of hydrated sodium halides NaX(H ₂ O)(1-6) (X=F, Cl, Br, and I). <i>Journal of Chemical Physics</i> , 2006 , 124, 024321	3.9	76
456	Nature of one-dimensional short hydrogen bonding: bond distances, bond energies, and solvent effects. <i>Journal of the American Chemical Society</i> , 2004 , 126, 2186-93	16.4	75
455	Ab Initio Study of the Structures, Energetics, and Spectra of Aquazinc(II). <i>The Journal of Physical Chemistry</i> , 1996 , 100, 14329-14338		74
454	Harmonic vibrational frequencies of the water monomer and dimer: Comparison of various levels of ab initio theory. <i>Journal of Chemical Physics</i> , 1995 , 102, 310-317	3.9	74
453	Benzene-hydrogen halide interactions: Theoretical studies of binding energies, vibrational frequencies, and equilibrium structures. <i>Journal of Chemical Physics</i> , 1998 , 108, 7217-7223	3.9	73
452	Control of the Plasmon in a single layer graphene by charge doping. <i>Applied Physics Letters</i> , 2011 , 99, 082110	3.4	72
451	Entropy-driven structures of the water octamer. <i>Chemical Physics Letters</i> , 1994 , 219, 243-246	2.5	72
450	Radioactive iodine capture and storage from water using magnetite nanoparticles encapsulated in polypyrrole. <i>Journal of Hazardous Materials</i> , 2018 , 344, 576-584	12.8	71
449	Interconnected Pt-nanodendrite/DNA/reduced-graphene-oxide hybrid showing remarkable oxygen reduction activity and stability. <i>ACS Nano</i> , 2013 , 7, 9223-31	16.7	71
448	Highly selective and stable carbon dioxide uptake in polyindole-derived microporous carbon materials. <i>Environmental Science & Technology</i> , 2013 , 47, 5467-73	10.3	71
447	Structures, energies, and vibrational spectra of water undecamer and dodecamer: An ab initio study. <i>Journal of Chemical Physics</i> , 2001 , 114, 10749-10756	3.9	71
446	Novel Amphi-Ionophores. <i>Journal of Physical Chemistry B</i> , 1998 , 102, 461-463	3.4	71
445	Ab initio molecular dynamics of liquid water using embedded-fragment second-order many-body perturbation theory towards its accurate property prediction. <i>Scientific Reports</i> , 2015 , 5, 14358	4.9	70
444	Fluorescent imidazolium-based cyclophane for detection of guanosine-5'-triphosphate and I(-) in aqueous solution of physiological pH. <i>Organic Letters</i> , 2011 , 13, 5476-9	6.2	70
443	2-dimensional analytic approach for anion differentiation with chromofluorogenic receptors. <i>Journal of Organic Chemistry</i> , 2007 , 72, 5461-4	4.2	70
442	Graphene-nanoplatelets-supported NiFe-MOF: high-efficiency and ultra-stable oxygen electrodes for sustained alkaline anion exchange membrane water electrolysis. <i>Energy and Environmental Science</i> , 2020 , 13, 3447-3458	35.4	69
441	Structures, energetics, and spectra of hydrated hydroxide anion clusters. <i>Journal of Chemical Physics</i> , 2004 , 121, 4657-64	3.9	69

440	Structural, electronic, and magnetic properties of a ferromagnetic semiconductor: Co-doped TiO ₂ rutile. <i>Physical Review B</i> , 2003 , 68,	3.3	69
439	Anisole-(H ₂ O) _n (n=1B) complexes: An experimental and theoretical investigation of the modulation of optimal structures, binding energies, and vibrational spectra in both the ground and first excited states. <i>Journal of Chemical Physics</i> , 2002 , 117, 8805-8822	3.9	69
438	Suppressed beta-hydride elimination in palladium-catalyzed cascade cyclization-coupling reactions: an efficient synthesis of 3-arylmethylpyrrolidines. <i>Organic Letters</i> , 2000 , 2, 1213-6	6.2	69
437	Reversible CO ₂ adsorption by an activated nitrogen doped graphene/polyaniline material. <i>Nanotechnology</i> , 2013 , 24, 235703	3.4	68
436	Prediction of reorganization free energies for biological electron transfer: a comparative study of Ru-modified cytochromes and a 4-helix bundle protein. <i>Journal of the American Chemical Society</i> , 2010 , 132, 17032-40	16.4	68
435	Structures and electronic properties of small carbon nanotube tori. <i>Physical Review B</i> , 2000 , 62, 1600-1603	6.3	67
434	Structure-mechanism-based engineering of chemical regulators targeting distinct pathological factors in Alzheimer's disease. <i>Nature Communications</i> , 2016 , 7, 13115	17.4	66
433	Designing Ionophores and Molecular Nanotubes Based on Molecular Recognition. <i>Supramolecular Chemistry</i> , 2007 , 19, 321-332	1.8	66
432	Superb water splitting activity of the electrocatalyst FeCo(PO) designed with computation aid. <i>Nature Communications</i> , 2019 , 10, 5195	17.4	65
431	Synthesis of single-crystal tetra(4-pyridyl)porphyrin rectangular nanotubes in the vapor phase. <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 2506-9	16.4	65
430	Vibrational spectra and electron detachment energy of the anionic water hexamer. <i>Journal of Chemical Physics</i> , 2000 , 113, 5273	3.9	65
429	Origin of the high affinity and selectivity of novel receptors for NH ₄ ⁺ over K ⁺ : charged hydrogen bonds vs cation- π interaction. <i>Organic Letters</i> , 2000 , 2, 2679-81	6.2	65
428	Extremely stable graphene electrodes doped with macromolecular acid. <i>Nature Communications</i> , 2018 , 9, 2037	17.4	65
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