Kwang S Kim

List of Publications by Year in Descending Order

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	Crystalline-amorphous interface of mesoporous Ni2P□@□FePOxHy for oxygen evolution at high current density in alkaline-anion-exchange-membrane water-electrolyzer. *Applied Catalysis B: Environmental*, **2022**, 306, 121127	21.8	11
582	Highly Efficient Pure-Blue Perovskite Light-Emitting Diode Leveraging CsPbBr x Cl 3□x /Cs 4 PbBr x Cl 6□x Nanocomposite Emissive Layer with Shallow V. *Advanced Optical Materials*, **2022**, 10, 2270024	8.1	
581	Unveiling the Role of Charge Transfer in Enhanced Electrochemical Nitrogen Fixation at Single-Atom Catalysts on BX Sheets (X = As, P, Sb).. *Journal of Physical Chemistry Letters*, **2022**, 4530-4537	6.4	4
580	Late Transition Metal Doped MXenes Showing Superb Bifunctional Electrocatalytic Activities for Water Splitting via Distinctive Mechanistic Pathways. *Advanced Energy Materials*, **2021**, 2102388	21.8	16
579	Perovskite solar cells with atomically coherent interlayers on SnO electrodes. *Nature*, **2021**, 598, 444-450	50.4	530
578	Machine Learning of First-Principles Force-Fields for Alkane and Polyene Hydrocarbons. *Journal of Physical Chemistry A*, **2021**, 125, 9414-9420	2.8	3
577	Supra-Binary Polarization in a Ferroelectric Nanowire. *Advanced Materials*, **2021**, 33, e2101981	24	1
576	Two Liquid-Liquid Phase Transitions in Confined Water Nanofilms. *Journal of Physical Chemistry Letters*, **2021**, 12, 4786-4792	6.4	2
575	Sparse Gaussian process potentials: Application to lithium diffusivity in superionic conducting solid electrolytes. *Physical Review B*, **2021**, 103,	3.3	14
574	Multi-site catalyst derived from Cr atoms-substituted CoFe nanoparticles for high-performance oxygen evolution activity. *Chemical Engineering Journal*, **2021**, 404, 126513	14.7	13
573	Anharmonicity-Driven Rashba Cohelical Excitons Break Quantum Efficiency Limitation. *Advanced Materials*, **2021**, 33, e2005400	24	1
572	Coarse and fine-tuning of lasing transverse electromagnetic modes in coupled all-inorganic perovskite quantum dots. *Nano Research*, **2021**, 14, 108-113	10	3
571	A universal screening strategy for the accelerated design of superior oxygen evolution/reduction electrocatalysts. *Journal of Materials Chemistry A*, **2021**, 9, 3511-3519	13	6
570	Na/Al Codoped Layered Cathode with Defects as Bifunctional Electrocatalyst for High-Performance Li-Ion Battery and Oxygen Evolution Reaction. *Small*, **2021**, 17, e2005605	11	7
569	Universal Machine Learning Interatomic Potentials: Surveying Solid Electrolytes. *Journal of Physical Chemistry Letters*, **2021**, 12, 8115-8120	6.4	14
568	Bifunctional oxovanadate doped cobalt carbonate for high-efficient overall water splitting in alkaline-anion-exchange-membrane water-electrolyzer. *Chemical Engineering Journal*, **2021**, 430, 132623	14.7	8
567	Ruthenium Core□Shell Engineering with Nickel Single Atoms for Selective Oxygen Evolution via Nondestructive Mechanism. *Advanced Energy Materials*, **2021**, 11, 2003448	21.8	44

566	Tuning metal single atoms embedded in NxCy moieties toward high-performance electrocatalysis. *Energy and Environmental Science*, **2021**, 14, 3455-3468	35.4	47
565	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	13	31
564	First principles and machine learning based superior catalytic activities and selectivities for N2 reduction in MBenes, defective 2D materials and 2D □-conjugated polymer-supported single atom catalysts. *Journal of Materials Chemistry A*, **2021**, 9, 9203-9213	13	9
563	Modulation of Cu and Rh single-atoms and nanoparticles for high-performance hydrogen evolution activity in acidic media. *Journal of Materials Chemistry A*, **2021**, 9, 10326-10334	13	19
562	Surface enrichment of iridium on IrCo alloys for boosting hydrogen production. *Journal of Materials Chemistry A*, **2021**, 9, 16898-16905	13	12
561	Recent Advancement of p- and d-Block Elements, Single Atoms, and Graphene-Based Photoelectrochemical Electrodes for Water Splitting. *Advanced Energy Materials*, **2020**, 10, 2000280	21.8	40
560	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	35.4	69
559	Interface Engineering Driven Stabilization of Halide Perovskites against Moisture, Heat, and Light for Optoelectronic Applications. *Advanced Energy Materials*, **2020**, 10, 2000768	21.8	32
558	Enhanced photoluminescence quantum yield of MAPbBr3 nanocrystals by passivation using graphene. *Nano Research*, **2020**, 13, 932-938	10	5
557	Machine Learning for Predicting the Band Gaps of ABX3 Perovskites from Elemental Properties. *Journal of Physical Chemistry C*, **2020**, 124, 8905-8918	3.8	36
556	Rational design of metal□gands for the conversion of CH4 and CO2 to acetates: role of acids and Lewis acids. *Journal of Materials Chemistry A*, **2020**, 8, 14671-14679	13	3
555	Machine learning-based high throughput screening for nitrogen fixation on boron-doped single atom catalysts. *Journal of Materials Chemistry A*, **2020**, 8, 5209-5216	13	47
554	Simple and Scalable Mechanochemical Synthesis of Noble Metal Catalysts with Single Atoms toward Highly Efficient Hydrogen Evolution. *Advanced Functional Materials*, **2020**, 30, 2000531	15.6	60
553	Multi-heteroatom-doped carbon from waste-yeast biomass for sustained water splitting. *Nature Sustainability*, **2020**, 3, 556-563	22.1	77
552	A high performance N-doped graphene nanoribbon based spintronic device applicable with a wide range of adatoms. *Nanoscale Advances*, **2020**, 2, 5905-5911	5.1	5
551	Accurate Description of Nuclear Quantum Effects with High-Order Perturbed Path Integrals (HOPPI). *Journal of Chemical Theory and Computation*, **2020**, 16, 1128-1135	6.4	6
550	Efficient electron extraction of SnO2 electron transport layer for lead halide perovskite solar cell. *Npj Computational Materials*, **2020**, 6,	10.9	10
549	Unfolding the Influence of Metal Doping on Properties of CsPbI3 Perovskite. *Small Methods*, **2020**, 4, 2000296	12.8	9

548	Perovskites: Interface Engineering Driven Stabilization of Halide Perovskites against Moisture, Heat, and Light for Optoelectronic Applications (Adv. Energy Mater. 30/2020). *Advanced Energy Materials*, **2020**, 10, 2070129	21.8	
547	Remarkably enhanced catalytic activity by the synergistic effect of palladium single atoms and palladium□cobalt phosphide nanoparticles. *Nano Energy*, **2020**, 78, 105166	17.1	28
546	Immiscible bi-metal single-atoms driven synthesis of electrocatalysts having superb mass-activity and durability. *Applied Catalysis B: Environmental*, **2020**, 270, 118896	21.8	44
545	A thermally stable, barium-stabilized □CsPbI3 perovskite for optoelectronic devices. *Journal of Materials Chemistry A*, **2019**, 7, 21740-21746	13	22
544	A "turn-on" fluorescent probe for the detection of permanganate in aqueous media. *Chemical Communications*, **2019**, 55, 1470-1473	5.8	8
543	Pt-like hydrogen evolution on a V2O5/Ni(OH)2 electrocatalyst. *Journal of Materials Chemistry A*, **2019**, 7, 15794-15800	13	21
542	High-Performance Hydrogen Evolution by Ru Single Atoms and Nitrided-Ru Nanoparticles Implanted on N-Doped Graphitic Sheet. *Advanced Energy Materials*, **2019**, 9, 1900931	21.8	131
541	Band Gap Narrowing of Zinc Orthogermanate by Dimensional and Defect Modification. *Journal of Physical Chemistry C*, **2019**, 123, 14573-14581	3.8	5
540	Effect of Organic□cation Exchange Reaction of Perovskites in Water: H-Bond Assisted Self-Assembly, Black Phase Stabilization, and Single-Particle Imaging. *ACS Applied Energy Materials*, **2019**, 2, 4496-4503	6.1	13
539	Compositional and Dimensional Control of 2D and Quasi-2D Lead Halide Perovskites in Water. *Advanced Functional Materials*, **2019**, 29, 1900966	15.6	24
538	Signature of a quantum dimensional transition in the spin-12 antiferromagnetic Heisenberg model on a square lattice and space reduction in the matrix product state. *Physical Review B*, **2019**, 99,	3.3	2
537	Single Atoms and Clusters Based Nanomaterials for Hydrogen Evolution, Oxygen Evolution Reactions, and Full Water Splitting. *Advanced Energy Materials*, **2019**, 9, 1900624	21.8	294
536	Multiphotoluminescence from a Triphenylamine Derivative and Its Application in White Organic Light-Emitting Diodes Based on a Single Emissive Layer. *Advanced Materials*, **2019**, 31, e1900613	24	19
535	First-order and continuous melting transitions in two-dimensional Lennard-Jones systems and repulsive disks. *Physical Review E*, **2019**, 99, 022145	2.4	12
534	Ideal conducting polymer anode for perovskite light-emitting diodes by molecular interaction decoupling. *Nano Energy*, **2019**, 60, 324-331	17.1	20
533	Quantum Monte Carlo Study of the Water Dimer Binding Energy and Halogen-□Interactions. *Journal of Physical Chemistry A*, **2019**, 123, 7785-7791	2.8	4
532	Dual Emission of Water-Stable 2D Organic□Inorganic Halide Perovskites with Mn(II) Dopant. *Advanced Functional Materials*, **2019**, 29, 1904768	15.6	45
531	An effective approach to realize graphene based p-n junctions via adsorption of donor and acceptor molecules. *Carbon*, **2019**, 153, 525-530	10.4	2

530	Superb water splitting activity of the electrocatalyst FeCo(PO) designed with computation aid. *Nature Communications*, **2019**, 10, 5195	17.4	65
529	Atomic scale study of black phosphorus degradation.. *RSC Advances*, **2019**, 10, 350-355	3.7	18
528	Signature of multilayer growth of 2D layered Bi2Se3 through heteroatom-assisted step-edge barrier reduction. *Npj 2D Materials and Applications*, **2019**, 3,	8.8	1
527	Formation of a photoactive quasi-2D formamidinium lead iodide perovskite in water. *Journal of Materials Chemistry A*, **2019**, 7, 25785-25790	13	9
526	Direct emission from quartet excited states triggered by upconversion phenomena in solid-phase synthesized fluorescent lead-free organic□inorganic hybrid compounds. *Journal of Materials Chemistry A*, **2019**, 7, 26504-26512	13	17
525	Selective separation of Xe/Kr and adsorption of water in a microporous hydrogen-bonded organic framework.. *RSC Advances*, **2019**, 9, 36808-36814	3.7	9
524	Non-adiabatic dynamics of ring opening in cyclohexa-1,3-diene described by an ensemble density-functional theory method. *Molecular Physics*, **2019**, 117, 1128-1141	1.7	26
523	A New Perspective on the Role of A-Site Cations in Perovskite Solar Cells. *Advanced Energy Materials*, **2018**, 8, 1702898	21.8	38
522	An ultra-sensitive, flexible and transparent gas detection film based on well-ordered flat polypyrrole on single-layered graphene. *Journal of Materials Chemistry A*, **2018**, 6, 2257-2263	13	25
521	Sulfur-vacancy-dependent geometric and electronic structure of bismuth adsorbed on MoS2. *Physical Review B*, **2018**, 97,	3.3	3
520	Anisotropic and amphoteric characteristics of diverse carbenes. *Physical Chemistry Chemical Physics*, **2018**, 20, 13722-13733	3.6	2
519	Radioactive iodine capture and storage from water using magnetite nanoparticles encapsulated in polypyrrole. *Journal of Hazardous Materials*, **2018**, 344, 576-584	12.8	71
518	Template free facile synthesis of mesoporous mordenite for bulky molecular catalytic reactions. *Journal of Industrial and Engineering Chemistry*, **2018**, 57, 363-369	6.3	10
517	Multicomponent electrocatalyst with ultralow Pt loading and high hydrogen evolution activity. *Nature Energy*, **2018**, 3, 773-782	62.3	330
516	Efficient separation of C hydrocarbons in a permanently porous hydrogen-bonded organic framework. *Chemical Communications*, **2018**, 54, 9360-9363	5.8	34
515	Direct Nonadiabatic Dynamics by Mixed Quantum-Classical Formalism Connected with Ensemble Density Functional Theory Method: Application to trans-Penta-2,4-dieniminium Cation. *Journal of Chemical Theory and Computation*, **2018**, 14, 4499-4512	6.4	27
514	Short-term Outcomes of Ceramic Coated Metal-on-Metal Large Head in Total Hip Replacement Arthroplasty. *Hip and Pelvis*, **2018**, 30, 12-17	1.5	3
513	Rashba□Dresselhaus Effect in Inorganic/Organic Lead Iodide Perovskite Interfaces. *ACS Energy Letters*, **2018**, 3, 1294-1300	20.1	30

512	Water-Stable, Fluorescent Organic–Inorganic Hybrid and Fully Inorganic Perovskites. *ACS Energy Letters*, **2018**, 3, 2120-2126	20.1	47
511	Fulgides as Light-Driven Molecular Rotary Motors: Computational Design of a Prototype Compound. *Journal of Physical Chemistry Letters*, **2018**, 9, 4995-5001	6.4	28
510	Intramolecular deformation of zeotype-borogermanate toward a three-dimensional porous germanium anode for high-rate lithium storage. *Journal of Materials Chemistry A*, **2018**, 6, 15961-15967	13	11
509	Organic cation steered interfacial electron transfer within organic–inorganic perovskite solar cells. *Journal of Materials Chemistry A*, **2018**, 6, 4305-4312	13	13
508	Synthesis of dual porous structured germanium anodes with exceptional lithium-ion storage performance. *Journal of Power Sources*, **2018**, 374, 217-224	8.9	28
507	La-doped BaSnO3 electron transport layer for perovskite solar cells. *Journal of Materials Chemistry A*, **2018**, 6, 23071-23077	13	26
506	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	36.5	78
505	Ambient-Stable Cubic-Phase Hybrid Perovskite Reaching the Shockley–Queisser Fill Factor Limit via Inorganic Additive-Assisted Process. *ACS Applied Energy Materials*, **2018**, 1, 5865-5871	6.1	10
504	Fuel Cells: Highly Efficient Oxygen Reduction Reaction Activity of Graphitic Tube Encapsulating Nitrided CoxFey Alloy (Adv. Energy Mater. 25/2018). *Advanced Energy Materials*, **2018**, 8, 1870115	21.8	4
503	A highly hydrophobic fluorographene-based system as an interlayer for electron transport in organic–inorganic perovskite solar cells. *Journal of Materials Chemistry A*, **2018**, 6, 18635-18640	13	18
502	Extremely stable graphene electrodes doped with macromolecular acid. *Nature Communications*, **2018**, 9, 2037	17.4	65
501	Perovskite Solar Cells: A New Perspective on the Role of A-Site Cations in Perovskite Solar Cells (Adv. Energy Mater. 14/2018). *Advanced Energy Materials*, **2018**, 8, 1870062	21.8	1
500	Turn-on and Turn-off Fluorescent Probes for Carbon Monoxide Detection and Blood Carboxyhemoglobin Determination. *ACS Sensors*, **2018**, 3, 1102-1108	9.2	33
499	Highly Efficient Oxygen Reduction Reaction Activity of Graphitic Tube Encapsulating Nitrided CoxFey Alloy. *Advanced Energy Materials*, **2018**, 8, 1801002	21.8	90
498	Two-Dimensional Excitonic Photoluminescence in Graphene on a Cu Surface. *ACS Nano*, **2017**, 11, 3207-3212	13.7	9
497	Size-dependent conformational change in halogen–π interaction: from benzene to graphene. *Chemical Communications*, **2017**, 53, 6140-6143	5.8	17
496	Mesoporous Silicon Hollow Nanocubes Derived from Metal-Organic Framework Template for Advanced Lithium-Ion Battery Anode. *ACS Nano*, **2017**, 11, 4808-4815	16.7	141
495	Interplay between many body effects and Coulomb screening in the optical bandgap of atomically thin MoS. *Nanoscale*, **2017**, 9, 10647-10652	7.7	13

494	Adsorption of Carbon Tetrahalides on Coronene and Graphene. *Journal of Physical Chemistry C*, **2017**, 121, 14968-14974	3.8	9
493	Structural and Mechanistic Insights into Development of Chemical Tools to Control Individual and Inter-Related Pathological Features in Alzheimer's Disease. *Chemistry - A European Journal*, **2017**, 23, 2706-2715	4.8	23
492	Efficient CO Oxidation by 50-Facet CuO Nanocrystals Coated with CuO Nanoparticles. *ACS Applied Materials & Interfaces*, **2017**, 9, 2495-2499	9.5	24
491	Accelerated Bone Regeneration by Two-Photon Photoactivated Carbon Nitride Nanosheets. *ACS Nano*, **2017**, 11, 742-751	16.7	56
490	Tunable Photoluminescence across the Visible Spectrum and Photocatalytic Activity of Mixed-Valence Rhenium Oxide Nanoparticles. *Journal of the American Chemical Society*, **2017**, 139, 15088-15093	14.4	21
489	Ferromagnetism in Monatomic Chains: Spin-Dependent Bandwidth Narrowing/Broadening. *Journal of Physical Chemistry C*, **2017**, 121, 20994-21000	3.8	7
488	Nickel-Based Electrocatalysts for Energy-Related Applications: Oxygen Reduction, Oxygen Evolution, and Hydrogen Evolution Reactions. *ACS Catalysis*, **2017**, 7, 7196-7225	13.1	568
487	High-Affinity-Assisted Nanoscale Alloys as Remarkable Bifunctional Catalyst for Alcohol Oxidation and Oxygen Reduction Reactions. *ACS Nano*, **2017**, 11, 7729-7735	16.7	79
486	Anomalous Ambipolar Transport of Organic Semiconducting Crystals via Control of Molecular Packing Structures. *ACS Applied Materials & Interfaces*, **2017**, 9, 27839-27846	9.5	9
485	Description of ground and excited electronic states by ensemble density functional method with extended active space. *Journal of Chemical Physics*, **2017**, 147, 064104	3.9	23
484	Graphene and Graphene Analogs toward Optical, Electronic, Spintronic, Green-Chemical, Energy-Material, Sensing, and Medical Applications. *ACS Applied Materials & Interfaces*, **2017**, 9, 24393-24406	9.5	45
483	Spectromicroscopic observation of a live single cell in a biocompatible liquid-enclosing graphene system. *Nanoscale*, **2017**, 10, 150-157	7.7	4
482	Two-Dimensional Icy Water Clusters Between a Pair of Graphene-Like Molecules or Graphene Sheets. *Journal of Physical Chemistry C*, **2016**, 120, 19212-19224	3.8	
481	Structure-mechanism-based engineering of chemical regulators targeting distinct pathological factors in Alzheimer's disease. *Nature Communications*, **2016**, 7, 13115	17.4	66
480	Water Splitting: One-Step Synthesis of CoS-Doped ‡Co(OH)2@Amorphous MoS2+x Hybrid Catalyst Grown on Nickel Foam for High-Performance Electrochemical Overall Water Splitting (Adv. Funct. Mater. 41/2016). *Advanced Functional Materials*, **2016**, 26, 7370-7370	15.6	3
479	Halogen-□Interactions between Benzene and X/CX (X = Cl, Br): Assessment of Various Density Functionals with Respect to CCSD(T). *Journal of Physical Chemistry A*, **2016**, 120, 9305-9314	2.8	29
478	Electron Transport in Graphene Nanoribbon Field-Effect Transistor under Bias and Gate Voltages: Isochemical Potential Approach. *Journal of Physical Chemistry Letters*, **2016**, 7, 2478-82	6.4	27
477	Covalent versus Charge Transfer Modification of Graphene/Carbon-Nanotubes with Vitamin B1: Co/N/S-C Catalyst toward Excellent Oxygen Reduction. *ACS Applied Materials & Interfaces*, **2016**, 8, 16045-52	9.5	29

476	An efficient non-reaction based colorimetric and fluorescent probe for the highly selective discrimination of Pd0 and Pd2+ in aqueous media. *RSC Advances*, **2016**, 6, 60546-60549	3.7	12
475	Effects of an electric field on interaction of aromatic systems. *Journal of Computational Chemistry*, **2016**, 37, 971-5	3.5	6
474	Using the GVB Ansatz to develop ensemble DFT method for describing multiple strongly correlated electron pairs. *Physical Chemistry Chemical Physics*, **2016**, 18, 21040-50	3.6	18
473	Functional molecules and materials by π interaction based quantum theoretical design. *International Journal of Quantum Chemistry*, **2016**, 116, 622-633	2.1	12
472	Antimony(III) Sulfide Thin Films as a Photoanode Material in Photocatalytic Water Splitting. *ACS Applied Materials & Interfaces*, **2016**, 8, 8445-51	9.5	47
471	Why Is MP2-Water "Cooler" and "Denser" than DFT-Water?. *Journal of Physical Chemistry Letters*, **2016**, 7, 680-4	6.4	39
470	Violation of DNA neighbor exclusion principle in RNA recognition. *Chemical Science*, **2016**, 7, 3581-3588	9.4	15
469	Cyanoacetic acid tethered thiophene for well-matched LUMO level in Ru(II)-terpyridine dye sensitized solar cells. *Dyes and Pigments*, **2016**, 126, 270-278	4.6	7
468	Engineered Carbon-Nanomaterial-Based Electrochemical Sensors for Biomolecules. *ACS Nano*, **2016**, 10, 46-80	16.7	337
467	Versatile p-Type Chemical Doping to Achieve Ideal Flexible Graphene Electrodes. *Angewandte Chemie - International Edition*, **2016**, 55, 6197-201	16.4	63
466	Versatile p-Type Chemical Doping to Achieve Ideal Flexible Graphene Electrodes. *Angewandte Chemie*, **2016**, 128, 6305-6309	3.6	7
465	Lower Electric Field-Driven Magnetic Phase Transition and Perfect Spin Filtering in Graphene Nanoribbons by Edge Functionalization. *Journal of Physical Chemistry Letters*, **2016**, 7, 5049-5055	6.4	31
464	Self-consistent implementation of ensemble density functional theory method for multiple strongly correlated electron pairs. *Journal of Chemical Physics*, **2016**, 145, 244104	3.9	21
463	Hemoglobin-carbon nanotube derived noble-metal-free Fe5C2-based catalyst for highly efficient oxygen reduction reaction. *Scientific Reports*, **2016**, 6, 20132	4.9	28
462	Observation of Mg-induced structural and electronic properties of graphene. *Applied Physics Letters*, **2016**, 109, 193104	3.4	2
461	Halides with Fifteen Aliphatic C-H⋯Anion Interaction Sites. *Scientific Reports*, **2016**, 6, 30123	4.9	5
460	Noncovalent Functionalization of Graphene and Graphene Oxide for Energy Materials, Biosensing, Catalytic, and Biomedical Applications. *Chemical Reviews*, **2016**, 116, 5464-519	68.1	1546
459	Band and bonding characteristics of N2+ ion-doped graphene. *RSC Advances*, **2016**, 6, 84959-84964	3.7	0

458	One-Step Synthesis of CoS-Doped Co(OH)2@Amorphous MoS2+x Hybrid Catalyst Grown on Nickel Foam for High-Performance Electrochemical Overall Water Splitting. *Advanced Functional Materials*, **2016**, 26, 7386-7393	15.6	166
457	Triazine-Based Microporous Polymers for Selective Adsorption of CO2. *Journal of Physical Chemistry C*, **2015**, 119, 5395-5402	3.8	64
456	A Facile Route for Patterned Growth of Metal-Insulator Carbon Lateral Junction through One-Pot Synthesis. *ACS Nano*, **2015**, 9, 8352-60	16.7	7
455	Graphene edges and beyond: temperature-driven structures and electromagnetic properties. *ACS Nano*, **2015**, 9, 4669-74	16.7	25
454	Geometrical and Electronic Characteristics of AunO2 (n = 2). *Journal of Physical Chemistry C*, **2015**, 150615095155002	3.8	10
453	Highly selective CO2 adsorption performance of carbazole based microporous polymers. *RSC Advances*, **2015**, 5, 41745-41750	3.7	13
452	Interactions of CO2 with various functional molecules. *Physical Chemistry Chemical Physics*, **2015**, 17, 10925-33	3.6	81
451	Tailoring Electronic and Magnetic Properties of MoS2 Nanotubes. *Journal of Physical Chemistry C*, **2015**, 119, 6405-6413	3.8	33
450	Clean Transfer of Wafer-Scale Graphene via Liquid Phase Removal of Polycyclic Aromatic Hydrocarbons. *ACS Nano*, **2015**, 9, 4726-33	16.7	54
449	Activated carbon derived from waste coffee grounds for stable methane storage. *Nanotechnology*, **2015**, 26, 385602	3.4	40
448	Disulfuric acid dissociated by two water molecules: ab initio and density functional theory calculations. *Physical Chemistry Chemical Physics*, **2015**, 17, 28556-64	3.6	2
447	Drift-induced modifications to the dynamical polarization of graphene. *Physical Review B*, **2015**, 92,	3.3	20
446	Hydrogenation-induced atomic stripes on the 2H MoS2 surface. *Physical Review B*, **2015**, 92,	3.3	26
445	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	4.9	70
444	Intriguing Electrostatic Potential of CO: Negative Bond-ends and Positive Bond-cylindrical-surface. *Scientific Reports*, **2015**, 5, 16307	4.9	25
443	Turn-On Ratiometric Fluorescent Probe for Selective Discrimination of Cr(3+) from Fe(3+) in Aqueous Media for Living Cell Imaging. *Chemistry - A European Journal*, **2015**, 21, 16349-53	4.8	18
442	Surface-Effect-Induced Optical Bandgap Shrinkage in GaN Nanotubes. *Nano Letters*, **2015**, 15, 4472-6	11.5	17
441	High-temperature in situ crystallographic observation of reversible gas sorption in impermeable organic cages. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 14156-61	11.5	25

440	Proximity Effect Induced Electronic Properties of Graphene on Bi□Te□Se. *ACS Nano*, **2015**, 9, 10861-6	16.7	31
439	Choosing a density functional for modeling adsorptive hydrogen storage: reference quantum mechanical calculations and a comparison of dispersion-corrected density functionals. *Physical Chemistry Chemical Physics*, **2015**, 17, 6423-32	3.6	27
438	Controllable n-type doping on CVD-grown single- and double-layer graphene mixture. *Advanced Materials*, **2015**, 27, 1619-23	24	38
437	Anisotropic charge distribution and anisotropic van der Waals radius leading to intriguing anisotropic noncovalent interactions. *Scientific Reports*, **2014**, 4, 5826	4.9	13
436	Noncovalent Functionalization of Graphene **2014**, 199-218		2
435	Novel ionophores with 2n-crown-n topology: anion sensing via pure aliphatic C-H□anion hydrogen bonding. *Organic Letters*, **2014**, 16, 334-7	6.2	17
434	Molecular sensing using armchair graphene nanoribbon. *Journal of Computational Chemistry*, **2014**, 35, 1916-20	3.5	15
433	Quasi-Free-Standing Graphene Monolayer on a Ni Crystal through Spontaneous Na Intercalation. *Physical Review X*, **2014**, 4,	9.1	10
432	Linear and nonlinear optical properties of indeno[2,1-b]fluorene and its structural isomers. *Physical Chemistry Chemical Physics*, **2014**, 16, 24592-7	3.6	12
431	Isoreticular MOFs based on a rhombic dodecahedral MOP as a tertiary building unit. *CrystEngComm*, **2014**, 16, 6391-6397	3.3	10
430	Spin-induced band modifications of graphene through intercalation of magnetic iron atoms. *Nanoscale*, **2014**, 6, 3824-9	7.7	43
429	Limit of metastability for liquid and vapor phases of water. *Physical Review Letters*, **2014**, 112, 157802	7.4	17
428	Density functional theory based study of molecular interactions, recognition, engineering, and quantum transport in □molecular systems. *Accounts of Chemical Research*, **2014**, 47, 3321-30	24.3	52
427	Two dimensional molecular electronics spectroscopy for molecular fingerprinting, DNA sequencing, and cancerous DNA recognition. *ACS Nano*, **2014**, 8, 1827-33	16.7	52
426	Inverse transfer method using polymers with various functional groups for controllable graphene doping. *ACS Nano*, **2014**, 8, 7968-75	16.7	23
425	Iron-oxide-supported nanocarbon in lithium-ion batteries, medical, catalytic, and environmental applications. *ACS Nano*, **2014**, 8, 7571-612	16.7	128
424	Simultaneous visualization of graphene grain boundaries and wrinkles with structural information by gold deposition. *ACS Nano*, **2014**, 8, 8662-8	16.7	53
423	Highly stable CO2/N2 and CO2/CH4 selectivity in hyper-cross-linked heterocyclic porous polymers. *ACS Applied Materials & Interfaces*, **2014**, 6, 7325-33	9.5	131

422	In Search of a Two-Dimensional Material for DNA Sequencing. *Journal of Physical Chemistry C*, **2014**, 118, 10855-10858	3.8	33
421	CO capture and conversion to HOCO radical by ionized water clusters. *Journal of Physical Chemistry A*, **2014**, 118, 7274-9	2.8	4
420	Persistent topological surface state at the interface of Bi2Se3 film grown on patterned graphene. *ACS Nano*, **2014**, 8, 1154-60	16.7	30
419	Precise tuning of cationic cyclophanes toward highly selective fluorogenic recognition of specific biophosphate anions. *Organic Letters*, **2014**, 16, 2150-3	6.2	48
418	Is the molecular Berry phase an artifact of the Born-Oppenheimer approximation?. *Physical Review Letters*, **2014**, 113, 263004	7.4	81
417	De Novo Design Theory: Nanomaterials and Molecular Devices **2014**, 1111-1120		
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