

Yong-Hyun Kim

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

125
papers

7,402
citations

44
h-index

84
g-index

130
ext. papers

8,175
ext. citations

9.7
avg, IF

5.91
L-index

#	Paper	IF	Citations
125	Hydrogen storage in novel organometallic buckyballs. <i>Physical Review Letters</i> , 2005 , 94, 155504	7.4	568
124	Suppression of Hydrogen Evolution Reaction in Electrochemical N ₂ Reduction Using Single-Atom Catalysts: A Computational Guideline. <i>ACS Catalysis</i> , 2018 , 8, 7517-7525	13.1	333
123	Single-atom catalysts for CO electroreduction with significant activity and selectivity improvements. <i>Chemical Science</i> , 2017 , 8, 1090-1096	9.4	319
122	Reversible Lithium-Ion Insertion in Molybdenum Oxide Nanoparticles. <i>Advanced Materials</i> , 2008 , 20, 3627-3632	7.3	304
121	Chemical structures of hydrazine-treated graphene oxide and generation of aromatic nitrogen doping. <i>Nature Communications</i> , 2012 , 3, 638	17.4	302
120	Theory, synthesis, and oxygen reduction catalysis of Fe-porphyrin-like carbon nanotube. <i>Physical Review Letters</i> , 2011 , 106, 175502	7.4	290
119	Nondissociative adsorption of H ₂ molecules in light-element-doped fullerenes. <i>Physical Review Letters</i> , 2006 , 96, 016102	7.4	283
118	Transparent conductive single-walled carbon nanotube networks with precisely tunable ratios of semiconducting and metallic nanotubes. <i>ACS Nano</i> , 2008 , 2, 1266-74	16.7	278
117	Workfunction-tunable, N-doped reduced graphene transparent electrodes for high-performance polymer light-emitting diodes. <i>ACS Nano</i> , 2012 , 6, 159-67	16.7	275
116	Steric-hindrance-driven shape transition in PbS quantum dots: understanding size-dependent stability. <i>Journal of the American Chemical Society</i> , 2013 , 135, 5278-81	16.4	242
115	Enhanced nanoscale friction on fluorinated graphene. <i>Nano Letters</i> , 2012 , 12, 6043-8	11.5	222
114	Tailored semiconducting carbon nanotube networks with enhanced thermoelectric properties. <i>Nature Energy</i> , 2016 , 1,	62.3	204
113	Effects of sulfur doping on graphene-based nanosheets for use as anode materials in lithium-ion batteries. <i>Journal of Power Sources</i> , 2014 , 262, 79-85	8.9	183
112	Ultrastable PbSe nanocrystal quantum dots via in situ formation of atomically thin halide adlayers on PbSe(100). <i>Journal of the American Chemical Society</i> , 2014 , 136, 8883-6	16.4	148
111	Electronic structure of radially deformed BN and BC ₃ nanotubes. <i>Physical Review B</i> , 2001 , 63,	3.3	142
110	Solid State Enabled Reversible Four Electron Storage. <i>Advanced Energy Materials</i> , 2013 , 3, 120-127	21.8	131
109	Ambient carbon dioxide capture by boron-rich boron nitride nanotube. <i>Journal of the American Chemical Society</i> , 2011 , 133, 2084-7	16.4	129

108	Enhancement of the anisotropic photocurrent in ferroelectric oxides by strain gradients. <i>Nature Nanotechnology</i> , 2015 , 10, 972-9	28.7	113
107	Defective fullerenes and nanotubes as molecular magnets: An ab initio study. <i>Physical Review B</i> , 2003 , 68,	3.3	107
106	Nanotribological Properties of Fluorinated, Hydrogenated, and Oxidized Graphenes. <i>Tribology Letters</i> , 2013 , 50, 137-144	2.8	104
105	Band-gap modification by radial deformation in carbon nanotubes. <i>Physical Review B</i> , 1999 , 60, 10656-10659	3.5	101
104	Intrinsic Photoluminescence Emission from Subdomained Graphene Quantum Dots. <i>Advanced Materials</i> , 2016 , 28, 5255-61	24	95
103	Dopant-specific unzipping of carbon nanotubes for intact crystalline graphene nanostructures. <i>Nature Communications</i> , 2016 , 7, 10364	17.4	94
102	Wiring-up hydrogenase with single-walled carbon nanotubes. <i>Nano Letters</i> , 2007 , 7, 3528-34	11.5	91
101	Divacancy-nitrogen-assisted transition metal dispersion and hydrogen adsorption in defective graphene: A first-principles study. <i>Physical Review B</i> , 2010 , 81,	3.3	79
100	Effect of spin state on the dihydrogen binding strength to transition metal centers in metal-organic frameworks. <i>Journal of the American Chemical Society</i> , 2007 , 129, 12606-7	16.4	77
99	Halide-Amine Co-Passivated Indium Phosphide Colloidal Quantum Dots in Tetrahedral Shape. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 3714-8	16.4	76
98	Selective and Regenerative Carbon Dioxide Capture by Highly Polarizing Porous Carbon Nitride. <i>ACS Nano</i> , 2015 , 9, 9148-57	16.7	73
97	Itinerant ferromagnetism in heterostructured C/BN nanotubes. <i>Physical Review B</i> , 2003 , 67,	3.3	72
96	Accurate and efficient calculation of van der Waals interactions within density functional theory by local atomic potential approach. <i>Journal of Chemical Physics</i> , 2008 , 129, 154102	3.9	70
95	Spectral correlation in incommensurate multiwalled carbon nanotubes. <i>Physical Review Letters</i> , 2003 , 90, 026601	7.4	60
94	Self-catalyzed hydrogenation and dihydrogen adsorption on titanium carbide nanoparticles. <i>Chemical Physics Letters</i> , 2006 , 425, 273-277	2.5	59
93	Dynamics of fullerene coalescence. <i>Physical Review Letters</i> , 2003 , 90, 065501	7.4	55
92	Subband mixing rules in circumferentially perturbed carbon nanotubes: Effects of transverse electric fields. <i>Physical Review B</i> , 2001 , 64,	3.3	54
91	First-Principles Prediction of Icosahedral Quantum Dots for Tetravalent Semiconductors. <i>Physical Review Letters</i> , 2004 , 93,	7.4	51

90	Monodisperse pattern nanoalloying for synergistic intermetallic catalysis. <i>Nano Letters</i> , 2013 , 13, 5720-6115	11.5	50
89	Switching and sensing spin states of co-porphyrin in bimolecular reactions on Au111 using scanning tunneling microscopy. <i>ACS Nano</i> , 2013 , 7, 9312-7	16.7	50
88	First-Principles Theory of Electrochemical Capacitance of Nanostructured Materials: Dipole-Assisted Subsurface Intercalation of Lithium in Pseudocapacitive TiO2 Anatase Nanosheets. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 4909-4915	3.8	48
87	Ab initio design of Ca-decorated organic frameworks for high capacity molecular hydrogen storage with enhanced binding. <i>Applied Physics Letters</i> , 2009 , 95, 033109	3.4	47
86	Divalent Fe Atom Coordination in Two-Dimensional Microporous Graphitic Carbon Nitride. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 25438-43	9.5	46
85	Enhancement of Friction by Water Intercalated between Graphene and Mica. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 3482-3487	6.4	45
84	Carrier-mediated long-range ferromagnetism in electron-doped Fe-C4 and Fe-N4 incorporated graphene. <i>Physical Review B</i> , 2012 , 86,	3.3	45
83	Is the Chain of Oxidation and Reduction Process Reversible in Luminescent Graphene Quantum Dots?. <i>Small</i> , 2015 , 11, 3773-81	11	44
82	Thermoelectric imaging of structural disorder in epitaxial graphene. <i>Nature Materials</i> , 2013 , 12, 913-8	27	44
81	Borane-modified graphene-based materials as CO2 adsorbents. <i>Carbon</i> , 2014 , 79, 450-456	10.4	42
80	High Performance Colloidal Quantum Dot Photovoltaics by Controlling Protic Solvents in Ligand Exchange. <i>Advanced Energy Materials</i> , 2017 , 7, 1700301	21.8	39
79	Complementary p- and n-type polymer doping for ambient stable graphene inverter. <i>ACS Nano</i> , 2014 , 8, 650-6	16.7	38
78	Generation of ultra-high-molecular-weight polyethylene from metallocenes immobilized onto N-doped graphene nanoplatelets. <i>Macromolecular Rapid Communications</i> , 2013 , 34, 533-8	4.8	36
77	Nanotube wires on commensurate InAs surfaces: binding energies, band alignments, and bipolar doping by the surfaces. <i>Physical Review Letters</i> , 2004 , 92, 176102	7.4	35
76	III-V colloidal nanocrystals: control of covalent surfaces. <i>Chemical Science</i> , 2019 , 11, 913-922	9.4	35
75	Accuracy of density functional theory methods for weakly bonded systems: The case of dihydrogen binding on metal centers. <i>Physical Review B</i> , 2010 , 82,	3.3	34
74	Hole-mediated hydrogen spillover mechanism in metal-organic frameworks. <i>Physical Review Letters</i> , 2010 , 104, 236101	7.4	31
73	N2-dopant of graphene with electrochemically switchable bifunctional ORR/OER catalysis for Zn-air battery. <i>Energy Storage Materials</i> , 2020 , 32, 517-524	19.4	30

72	Ab initio calculations predicting the existence of an oxidized calcium dihydrogen complex to store molecular hydrogen in densities up to 100 g/L. <i>Physical Review B</i> , 2009 , 79,	3.3	28
71	Extremely Stable Luminescent Crosslinked Perovskite Nanoparticles under Harsh Environments over 1.5 Years. <i>Advanced Materials</i> , 2021 , 33, e2005255	24	26
70	Effect of chemical bonding on the magnetic stability and magnetic moment in Mn-based binary compounds. <i>Physical Review B</i> , 2005 , 72,	3.3	25
69	Gold nanoparticle-doped graphene nanosheets: sub-nanosized gold clusters nucleate and grow at the nitrogen-induced defects on graphene surfaces. <i>Journal of Materials Chemistry</i> , 2012 , 22, 7130		24
68	Persistent medium-range order and anomalous liquid properties of Al(1-x)Cu(x) alloys. <i>Physical Review Letters</i> , 2012 , 108, 115901	7.4	24
67	Self-assembly of linear arrays of semiconductor nanoparticles on carbon single-walled nanotubes. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 25153-7	3.4	24
66	Progress in Computational and Machine-Learning Methods for Heterogeneous Small-Molecule Activation. <i>Advanced Materials</i> , 2020 , 32, e1907865	24	23
65	Seebeck effect at the atomic scale. <i>Physical Review Letters</i> , 2014 , 112, 136601	7.4	23
64	Origin of the diverse melting behaviors of intermediate-size nanoclusters: theoretical study of AlN (N = 51-58, 64). <i>Journal of the American Chemical Society</i> , 2010 , 132, 18287-91	16.4	23
63	Dielectric-screening properties and Coulomb pseudopotential μ for MgB ₂ . <i>Physical Review B</i> , 2004 , 70,	3.3	23
62	Growth Mechanism of Catalyst-Free and Mask-Free Heteroepitaxial GaN Submicrometer- and Micrometer-Sized Rods under Biaxial Strain: Variation of Surface Energy and Adatom Kinetics. <i>Crystal Growth and Design</i> , 2012 , 12, 3838-3844	3.5	22
61	Finite-temperature hydrogen adsorption and desorption thermodynamics driven by soft vibration modes. <i>Physical Review Letters</i> , 2013 , 111, 066102	7.4	22
60	Opening space for H ₂ storage: Cointercalation of graphite with lithium and small organic molecules. <i>Physical Review B</i> , 2008 , 78,	3.3	22
59	Shape control of Al nanoclusters by ligand size. <i>Journal of the American Chemical Society</i> , 2009 , 131, 8522-6	16.4	21
58	Enhanced dihydrogen adsorption in symmetry-lowered metal-porphyrin-containing frameworks. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 11400-3	3.6	21
57	Electronic structure of collapsed C, BN, and BC ₃ nanotubes. <i>Current Applied Physics</i> , 2001 , 1, 39-44	2.6	21
56	Origin of the Stability and Transition from Anionic to Cationic Surface Ligand Passivation of All-Inorganic Cesium Lead Halide Perovskite Nanocrystals. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 652-658	6.4	21
55	Slow colloidal growth of PbSe nanocrystals for facile morphology and size control. <i>RSC Advances</i> , 2014 , 4, 9842	3.7	20

54	Atomically abrupt liquid-oxide interface stabilized by self-regulated interfacial defects: the case of Al/Al ₂ O ₃ interfaces. <i>Physical Review Letters</i> , 2012 , 108, 226105	7.4	20
53	Cyclodextrin driven hydrophobic/hydrophilic transformation of semiconductor nanoparticles. <i>Applied Physics Letters</i> , 2005 , 86, 033108	3.4	20
52	Nanoscale Friction on Confined Water Layers Intercalated between MoS ₂ Flakes and Silica. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 8827-8835	3.8	19
51	The Effect of Thickness and Chemical Reduction of Graphene Oxide on Nanoscale Friction. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 543-547	3.4	18
50	>1000-Fold Lifetime Extension of a Nickel Electromechanical Contact Device via Graphene. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 9085-9093	9.5	17
49	Comment on "Inaccuracy of density functional theory calculations for dihydrogen binding energetics onto Ca cation centers". <i>Physical Review Letters</i> , 2010 , 104, 179601; author reply 179602	7.4	17
48	Microscopic theory of hysteretic hydrogen adsorption in nanoporous materials. <i>Journal of the American Chemical Society</i> , 2010 , 132, 1510-1	16.4	17
47	Atomic models for anionic ligand passivation of cation-rich surfaces of IV-VI, II-VI, and III-V colloidal quantum dots. <i>Chemical Communications</i> , 2016 , 53, 388-391	5.8	16
46	Isotope- and Thickness-Dependent Friction of Water Layers Intercalated Between Graphene and Mica. <i>Tribology Letters</i> , 2018 , 66, 1	2.8	16
45	Phase diagram of graphene nanoribbons and band-gap bifurcation of Dirac fermions under quantum confinement. <i>Physical Review B</i> , 2012 , 85,	3.3	15
44	Half-solidity of tetrahedral-like Al(55) clusters. <i>ACS Nano</i> , 2010 , 4, 1092-8	16.7	14
43	Thickness-dependent photocatalytic performance of graphite oxide for degrading organic pollutants under visible light. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 10882-6	3.6	13
42	First-Principles Study of Electronic Structure and Hydrogen Adsorption of 3d Transition Metal Exposed Paddle Wheel Frameworks. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 7386-7392	3.8	13
41	Interfacial thermal conductance observed to be higher in semiconducting than metallic carbon nanotubes. <i>ACS Nano</i> , 2012 , 6, 3853-60	16.7	13
40	Halide/Amine Co-Passivated Indium Phosphide Colloidal Quantum Dots in Tetrahedral Shape. <i>Angewandte Chemie</i> , 2016 , 128, 3778-3782	3.6	13
39	Selective engineering of oxygen-containing functional groups using the alkyl ligand oleylamine for revealing the luminescence mechanism of graphene oxide quantum dots. <i>Nanoscale</i> , 2017 , 9, 18635-18643	7.7	12
38	Origin of enhanced dihydrogen-metal interaction in carboxylate bridged Cu ₂ -paddle-wheel frameworks. <i>Physical Review Letters</i> , 2010 , 105, 236105	7.4	12
37	O, NO and NH coordination to Co-porphyrin studied with scanning tunneling microscopy on Au(111). <i>Nanoscale</i> , 2019 , 11, 8510-8517	7.7	11

36	Visualizing tilted binding and precession of diatomic NO adsorbed to Co-porphyrin on Au(111) using scanning tunneling microscopy. <i>Chemical Science</i> , 2014 , 5, 2224-2229	9.4	11
35	Raman spectroscopy of charge transfer interactions between single wall carbon nanotubes and [FeFe] hydrogenase. <i>Dalton Transactions</i> , 2008 , 5454-61	4.3	11
34	Probing Single-Molecule Dissociations from a Bimolecular Complex NO-Co-Porphyrin. <i>ACS Nano</i> , 2015 , 9, 7722-8	16.7	10
33	Hysteresis and Photoinstability Caused by Mobile Ions in Colloidal Quantum Dot Photovoltaics. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 5259-5263	6.4	9
32	Altering the spin state of transition metal centers in metal-organic frameworks by molecular hydrogen adsorption: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 5042-6	3.6	9
31	Dihydrogen bonding, p-type conductivity, and origin of change in work function of hydrogenated diamond (001) surfaces. <i>Physical Review B</i> , 2006 , 74,	3.3	9
30	Origin of High-TC Ferromagnetism in Isovalent-Doped III-V Semiconductors. <i>Physical Review Applied</i> , 2019 , 11,	4.3	8
29	Anomalous Defect Dependence of Thermal Conductivity in Epitaxial WO Thin Films. <i>Advanced Materials</i> , 2019 , 31, e1903738	24	8
28	First-principles calculation of thermodynamic stability of acids and bases under pH environment: a microscopic pH theory. <i>Journal of Chemical Physics</i> , 2012 , 136, 134112	3.9	8
27	Coordination structure of Jacobsen catalyst with N-modified graphene and their electrocatalytic properties for reducing oxygen molecules. <i>Applied Catalysis B: Environmental</i> , 2020 , 263, 118337	21.8	8
26	Axial coordination and electronic structure of diatomic NO, CO, and O molecules adsorbed onto Co-tetraphenylporphyrin on Au(111), Ag(111), and Cu(111): a density-functional theory study. <i>Dalton Transactions</i> , 2016 , 45, 16673-16681	4.3	8
25	Microscopic States and the Verwey Transition of Magnetite Nanocrystals Investigated by Nuclear Magnetic Resonance. <i>Nano Letters</i> , 2018 , 18, 1745-1750	11.5	7
24	Amorphous Mixture of Two Indium-Free BaSnO and ZnSnO for Thin-Film Transistors with Balanced Performance and Stability. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 3719-3726	9.5	7
23	Tuning and sensing spin interactions in Co-porphyrin/Au with NH ₃ and NO ₂ binding. <i>Physical Review B</i> , 2019 , 100,	3.3	7
22	Reversible oxidation states of single layer graphene tuned by electrostatic potential. <i>Surface Science</i> , 2013 , 612, 37-41	1.8	6
21	Shape-controlled syntheses of metal oxide nanoparticles by the introduction of rare-earth metals. <i>Nanoscale</i> , 2017 , 9, 2732-2738	7.7	6
20	Origin of anomalous strain effects on the molecular adsorption on boron-doped graphene. <i>Journal of Chemical Physics</i> , 2013 , 139, 044709	3.9	6
19	Growing extremely thin bulklike metal film on a semiconductor surface: Monolayer Al(111) on Si(111). <i>Applied Physics Letters</i> , 2007 , 91, 181902	3.4	6

18	Tailoring graphene magnetism by zigzag triangular holes: A first-principles thermodynamics study. <i>AIP Advances</i> , 2016 , 6, 035023	1.5	6
17	Bimodal Control of Heat Transport at Graphene-Metal Interfaces Using Disorder in Graphene. <i>Scientific Reports</i> , 2016 , 6, 34428	4.9	5
16	Harnessing the topotactic transition in oxide heterostructures for fast and high-efficiency electrochromic applications. <i>Science Advances</i> , 2020 , 6,	14.3	5
15	Tailored growth of single-crystalline InP tetrapods. <i>Nature Communications</i> , 2021 , 12, 4454	17.4	5
14	Assessing the Predictive Power of Density Functional Theory in Finite-Temperature Hydrogen Adsorption/Desorption Thermodynamics. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 26189-26195	3.8	4
13	Quantitative Analysis of Calcium Phosphate Nanocluster Growth Using Time-of-Flight Medium-Energy-Ion-Scattering Spectroscopy. <i>ACS Central Science</i> , 2018 , 4, 1253-1260	16.8	4
12	Tip-Induced Strain Engineering of a Single Metal Halide Perovskite Quantum Dot. <i>ACS Nano</i> , 2021 , 15, 9057-9064	16.7	3
11	Ni Nanoparticles on Ni Core/N-Doped Carbon Shell Heterostructures for Electrocatalytic Oxygen Evolution. <i>ACS Applied Nano Materials</i> , 2021 , 4, 9418-9429	5.6	3
10	Spectral properties of incommensurate double-walled carbon nanotubes. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2004 , 22, 666-669	3	2
9	Importance of Turning to Renewable Energy Resources with Hydrogen as a Promising Candidate and on-board Storage a Critical Barrier. <i>Materials Research Society Symposia Proceedings</i> , 2005 , 895, 1		2
8	Electron transport through quantum-dot states of n-type carbon nanotubes. <i>Applied Physics Letters</i> , 2002 , 81, 2264-2266	3.4	2
7	Influence of the metal phthalocyanine molecular orientation on charge separation at the organic donor/acceptor interface. <i>Journal of Materials Chemistry C</i> , 2021 , 9, 2156-2164	7.1	1
6	Energy Storage: Hydrogen 2013 , 131-148		
5	Hydrogen Storage in Novel Carbon-Based Nanostructured Materials. <i>Materials Research Society Symposia Proceedings</i> , 2006 , 927, 1		
4	Novel Organometallic Fullerene Complexes for Vehicular Hydrogen Storage. <i>Materials Research Society Symposia Proceedings</i> , 2007 , 1041, 1		
3	Cyclodextrins Stabilize TOPO-(CdSe)ZnS Quantum Dots in Water. <i>Materials Research Society Symposia Proceedings</i> , 2004 , 823, W4.5.1		
2	Generalized Kubas Complexes as a Novel Means for Room Temperature Molecular Hydrogen Storage. <i>Materials Research Society Symposia Proceedings</i> , 2004 , 837, 63		
1	Perovskite Nanoparticles: Extremely Stable Luminescent Crosslinked Perovskite Nanoparticles under Harsh Environments over 1.5 Years (Adv. Mater. 3/2021). <i>Advanced Materials</i> , 2021 , 33, 2170017	24	

