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	Bifunctional oxovanadate doped cobalt carbonate for high-efficient overall water splitting in alkaline-anion-exchange-membrane water-electrolyzer. Chemical Engineering Journal, 2022, 430, 132623.	6.6	58
2	Machine learning assisted high-throughput screening of transition metal single atom based superb hydrogen evolution electrocatalysts. Journal of Materials Chemistry A, 2022, 10, 6679-6689.	5.2	74
3	Highly Efficient Pureâ€Blue Perovskite Lightâ€Emitting Diode Leveraging CsPbBr_xCl_{3â^'}_x/Cs₄PbBr_xCl_{6â^'}_x Nanocomposite Emissive Layer with Shallow Valence Band. Advanced Optical Materials, 2022, 10, .	8.6	6
4	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
5	Sparse Gaussian Process Regression-Based Machine Learned First-Principles Force-Fields for Saturated, Olefinic, and Aromatic Hydrocarbons. ACS Physical Chemistry Au, 2022, 2, 260-264.	1.9	5
6	Highly Efficient Pureâ€Blue Perovskite Lightâ€Emitting Diode Leveraging CsPbBr_xCl_{3â^'}_x/Cs₄PbBr_xCl_{6â^'}_x Nanocomposite Emissive Layer with Shallow Valence Band (Advanced Optical Materials 6/2022). Advanced Optical Materials, 2022, 10, .	8.6	0
7	C₆₀ Adsorbed on TiO₂ Drives Dark Generation of Hydroxyl Radicals. ACS Catalysis, 2022, 12, 5990-5996.	5.5	5
8	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, 13, 4530-4537.	2.1	29
9	Fast atomic structure optimization with on-the-fly sparse Gaussian process potentials [*]. Journal of Physics Condensed Matter, 2022, 34, 344007.	0.7	2
10	Alâ€Doping Driven Suppression of Capacity and Voltage Fadings in 4dâ€Element Containing Liâ€Ionâ€Battery Cathode Materials: Machine Learning and Density Functional Theory. Advanced Energy Materials, 2022, 12, .	10.2	42
11	Multi-site catalyst derived from Cr atoms-substituted CoFe nanoparticles for high-performance oxygen evolution activity. Chemical Engineering Journal, 2021, 404, 126513.	6.6	41
12	Anharmonicityâ€Driven Rashba Cohelical Excitons Break Quantum Efficiency Limitation. Advanced Materials, 2021, 33, 2005400.	11.1	1
13	Coarse and fine-tuning of lasing transverse electromagnetic modes in coupled all-inorganic perovskite quantum dots. Nano Research, 2021, 14, 108-113.	5.8	5
14	Facile room-temperature self-assembly of extended cation-free guanine-quartet network on Mo-doped Au(111) surface. Nanoscale Advances, 2021, 3, 3867-3874.	2.2	2
15	A universal screening strategy for the accelerated design of superior oxygen evolution/reduction electrocatalysts. Journal of Materials Chemistry A, 2021, 9, 3511-3519.	5.2	21
16	Na/Al Codoped Layered Cathode with Defects as Bifunctional Electrocatalyst for Highâ€Performance Liâ€Ion Battery and Oxygen Evolution Reaction. Small, 2021, 17, e2005605.	5.2	31
17	Supraâ€Binary Polarization in a Ferroelectric Nanowire. Advanced Materials, 2021, 33, e2101981.	11.1	4
18	Two Liquidâ€“Liquid Phase Transitions in Confined Water Nanofilms. Journal of Physical Chemistry Letters, 2021, 12, 4786-4792.	2.1	4

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19	Sparse Gaussian process potentials: Application to lithium diffusivity in superionic conducting solid electrolytes. Physical Review B, 2021, 103, .	1.1	41
20	Universal Machine Learning Interatomic Potentials: Surveying Solid Electrolytes. Journal of Physical Chemistry Letters, 2021, 12, 8115-8120.	2.1	45
21	Ruthenium Coreâ€“Shell Engineering with Nickel Single Atoms for Selective Oxygen Evolution via Nondestructive Mechanism. Advanced Energy Materials, 2021, 11, 2003448.	10.2	124
22	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
23	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
24	First principles and machine learning based superior catalytic activities and selectivities for N₂ reduction in MBenes, defective 2D materials and 2D Ï€-conjugated polymer-supported single atom catalysts. Journal of Materials Chemistry A, 2021, 9, 9203-9213.	5.2	67
25	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.	5.2	70
26	Surface enrichment of iridium on IrCo alloys for boosting hydrogen production. Journal of Materials Chemistry A, 2021, 9, 16898-16905.	5.2	65
27	Perovskite solar cells with atomically coherent interlayers on SnO2 electrodes. Nature, 2021, 598, 444-450.	13.7	2,065
28	Machine Learning of First-Principles Force-Fields for Alkane and Polyene Hydrocarbons. Journal of Physical Chemistry A, 2021, 125, 9414-9420.	1.1	19
29	Late Transition Metal Doped MXenes Showing Superb Bifunctional Electrocatalytic Activities for Water Splitting via Distinctive Mechanistic Pathways. Advanced Energy Materials, 2021, 11, 2102388.	10.2	73
30	Accurate Description of Nuclear Quantum Effects with High-Order Perturbed Path Integrals (HOPPI). Journal of Chemical Theory and Computation, 2020, 16, 1128-1135.	2.3	7
31	Atomic scale study of black phosphorus degradation. RSC Advances, 2020, 10, 350-355.	1.7	25
32	Efficient electron extraction of SnO2 electron transport layer for lead halide perovskite solar cell. Npj Computational Materials, 2020, 6, .	3.5	42
33	Unfolding the Influence of Metal Doping on Properties of CsPbI₃ Perovskite. Small Methods, 2020, 4, 2000296.	4.6	27
34	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.	10.2	1
35	Remarkably enhanced catalytic activity by the synergistic effect of palladium single atoms and palladiumâ€“cobalt phosphide nanoparticles. Nano Energy, 2020, 78, 105166.	8.2	57
36	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

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37	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
38	Interface Engineering Driven Stabilization of Halide Perovskites against Moisture, Heat, and Light for Optoelectronic Applications. Advanced Energy Materials, 2020, 10, 2000768.	10.2	62
39	Enhanced photoluminescence quantum yield of MAPbBr3 nanocrystals by passivation using graphene. Nano Research, 2020, 13, 932-938.	5.8	11
40	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
41	Rational design of metalâ€“ligands for the conversion of CH₄ and CO₂ to acetates: role of acids and Lewis acids. Journal of Materials Chemistry A, 2020, 8, 14671-14679.	5.2	7
42	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
43	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
44	Multi-heteroatom-doped carbon from waste-yeast biomass for sustained water splitting. Nature Sustainability, 2020, 3, 556-563.	11.5	186
45	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
46	A high performance N-doped graphene nanoribbon based spintronic device applicable with a wide range of adatoms. Nanoscale Advances, 2020, 2, 5905-5911.	2.2	10
47	Quantum Monte Carlo Study of the Water Dimer Binding Energy and Halogenâ˜Ï€ Interactions. Journal of Physical Chemistry A, 2019, 123, 7785-7791.	1.1	5
48	Dual Emission of Waterâ€Stable 2D Organicâ€“Inorganic Halide Perovskites with Mn(II) Dopant. Advanced Functional Materials, 2019, 29, 1904768.	7.8	66
49	An effective approach to realize graphene based p-n junctions via adsorption of donor and acceptor molecules. Carbon, 2019, 153, 525-530.	5.4	6
50	Superb water splitting activity of the electrocatalyst Fe3Co(PO4)4 designed with computation aid. Nature Communications, 2019, 10, 5195.	5.8	120
51	A thermally stable, barium-stabilized Î±-CsPbI₃ perovskite for optoelectronic devices. Journal of Materials Chemistry A, 2019, 7, 21740-21746.	5.2	37
52	A â€œturn-onâ€•fluorescent probe for the detection of permanganate in aqueous media. Chemical Communications, 2019, 55, 1470-1473.	2.2	20
53	Pt-like hydrogen evolution on a V₂O₅/Ni(OH)₂ electrocatalyst. Journal of Materials Chemistry A, 2019, 7, 15794-15800.	5.2	31
54	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

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55	Band Gap Narrowing of Zinc Orthogermanate by Dimensional and Defect Modification. Journal of Physical Chemistry C, 2019, 123, 14573-14581.	1.5	6
56	Effect of Organicâ€“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.	2.5	19
57	Compositional and Dimensional Control of 2D and Quasiâ€2D Lead Halide Perovskites in Water. Advanced Functional Materials, 2019, 29, 1900966.	7.8	27
58	Signature of a quantum dimensional transition in the spin- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mfrac><mml:mn>1</mml:mn><mml:mn>2</mml:mn></mml:mfrac></mml antiferromagnetic Heisenberg model on a square lattice and space reduction in the matrix product state. Physical Review B, 2019, 99, .	1.1	2
59	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
60	Multiphotoluminescence from a Triphenylamine Derivative and Its Application in White Organic Lightâ€Emitting Diodes Based on a Single Emissive Layer. Advanced Materials, 2019, 31, e1900613.	11.1	25
61	First-order and continuous melting transitions in two-dimensional Lennard-Jones systems and repulsive disks. Physical Review E, 2019, 99, 022145.	0.8	18
62	Ideal conducting polymer anode for perovskite light-emitting diodes by molecular interaction decoupling. Nano Energy, 2019, 60, 324-331.	8.2	28
63	Signature of multilayer growth of 2D layered Bi2Se3 through heteroatom-assisted step-edge barrier reduction. Npj 2D Materials and Applications, 2019, 3, .	3.9	1
64	Formation of a photoactive quasi-2D formamidinium lead iodide perovskite in water. Journal of Materials Chemistry A, 2019, 7, 25785-25790.	5.2	24
65	Direct emission from quartet excited states triggered by upconversion phenomena in solid-phase synthesized fluorescent lead-free organicâ€“inorganic hybrid compounds. Journal of Materials Chemistry A, 2019, 7, 26504-26512.	5.2	35
66	Selective separation of Xe/Kr and adsorption of water in a microporous hydrogen-bonded organic framework. RSC Advances, 2019, 9, 36808-36814.	1.7	28
67	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.	0.8	33
68	A New Perspective on the Role of Aâ€Site Cations in Perovskite Solar Cells. Advanced Energy Materials, 2018, 8, 1702898.	10.2	47
69	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.	5.2	33
70	Sulfur-vacancy-dependent geometric and electronic structure of bismuth adsorbed on <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mo</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2018, 97, .	1.1	4
71	Anisotropic and amphoteric characteristics of diverse carbenes. Physical Chemistry Chemical Physics, 2018, 20, 13722-13733.	1.3	4
72	Radioactive iodine capture and storage from water using magnetite nanoparticles encapsulated in polypyrrole. Journal of Hazardous Materials, 2018, 344, 576-584.	6.5	120

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73	Template free facile synthesis of mesoporous mordenite for bulky molecular catalytic reactions. Journal of Industrial and Engineering Chemistry, 2018, 57, 363-369.	2.9	13
74	Organic cation steered interfacial electron transfer within organicâ€“inorganic perovskite solar cells. Journal of Materials Chemistry A, 2018, 6, 4305-4312.	5.2	15
75	Synthesis of dual porous structured germanium anodes with exceptional lithium-ion storage performance. Journal of Power Sources, 2018, 374, 217-224.	4.0	33
76	Spectromicroscopic observation of a live single cell in a biocompatible liquid-enclosing graphene system. Nanoscale, 2018, 10, 150-157.	2.8	4
77	La-doped BaSnO₃ electron transport layer for perovskite solar cells. Journal of Materials Chemistry A, 2018, 6, 23071-23077.	5.2	37
78	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
79	Ambient-Stable Cubic-Phase Hybrid Perovskite Reaching the Shockleyâ€“Queisser Fill Factor Limit via Inorganic Additive-Assisted Process. ACS Applied Energy Materials, 2018, 1, 5865-5871.	2.5	13
80	Fuel Cells: Highly Efficient Oxygen Reduction Reaction Activity of Graphitic Tube Encapsulating Nitrided Co_xFe_y Alloy (Adv. Energy Mater. 25/2018). Advanced Energy Materials, 2018, 8, 1870115.	10.2	5
81	A highly hydrophobic fluorographene-based system as an interlayer for electron transport in organicâ€“inorganic perovskite solar cells. Journal of Materials Chemistry A, 2018, 6, 18635-18640.	5.2	20
82	Extremely stable graphene electrodes doped with macromolecular acid. Nature Communications, 2018, 9, 2037.	5.8	96
83	Perovskite Solar Cells: A New Perspective on the Role of A-Site Cations in Perovskite Solar Cells (Adv.) Tj ETQq1 1 0.784314 rgBT /Ove	10.2	1
84	Turn-on and Turn-off Fluorescent Probes for Carbon Monoxide Detection and Blood Carboxyhemoglobin Determination. ACS Sensors, 2018, 3, 1102-1108.	4.0	44
85	Highly Efficient Oxygen Reduction Reaction Activity of Graphitic Tube Encapsulating Nitrided Co_xFe_y Alloy. Advanced Energy Materials, 2018, 8, 1801002.	10.2	117
86	Multicomponent electrocatalyst with ultralow Pt loading and high hydrogen evolution activity. Nature Energy, 2018, 3, 773-782.	19.8	542
87	Efficient separation of C₂ hydrocarbons in a permanently porous hydrogen-bonded organic framework. Chemical Communications, 2018, 54, 9360-9363.	2.2	58
88	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.	2.3	30
89	Short-term Outcomes of Ceramic Coated Metal-on-Metal Large Head in Total Hip Replacement Arthroplasty. Hip and Pelvis, 2018, 30, 12-17.	0.6	4
90	Rashbaâ€“Dresselhaus Effect in Inorganic/Organic Lead Iodide Perovskite Interfaces. ACS Energy Letters, 2018, 3, 1294-1300.	8.8	36

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91	Water-Stable, Fluorescent Organicâ˜Inorganic Hybrid and Fully Inorganic Perovskites. ACS Energy Letters, 2018, 3, 2120-2126.	8.8	65
92	Fulgides as Light-Driven Molecular Rotary Motors: Computational Design of a Prototype Compound. Journal of Physical Chemistry Letters, 2018, 9, 4995-5001.	2.1	48
93	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.	5.2	17
94	Two-Dimensional Excitonic Photoluminescence in Graphene on a Cu Surface. ACS Nano, 2017, 11, 3207-3212.	7.3	11
95	Size-dependent conformational change in halogenâ€“Ï€ interaction: from benzene to graphene. Chemical Communications, 2017, 53, 6140-6143.	2.2	19
96	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
97	Interplay between many body effects and Coulomb screening in the optical bandgap of atomically thin MoS₂. Nanoscale, 2017, 9, 10647-10652.	2.8	23
98	Adsorption of Carbon Tetrahalides on Coronene and Graphene. Journal of Physical Chemistry C, 2017, 121, 14968-14974.	1.5	11
99	Structural and Mechanistic Insights into Development of Chemical Tools to Control Individual and Interâ€Related Pathological Features in Alzheimer's Disease. Chemistry - A European Journal, 2017, 23, 2706-2715.	1.7	25
100	Efficient CO Oxidation by 50-Facet Cu₂O Nanocrystals Coated with CuO Nanoparticles. ACS Applied Materials & Interfaces, 2017, 9, 2495-2499.	4.0	31
101	Accelerated Bone Regeneration by Two-Photon Photoactivated Carbon Nitride Nanosheets. ACS Nano, 2017, 11, 742-751.	7.3	78
102	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.	6.6	33
103	Ferromagnetism in Monatomic Chains: Spin-Dependent Bandwidth Narrowing/Broadening. Journal of Physical Chemistry C, 2017, 121, 20994-21000.	1.5	8
104	Nickel-Based Electrocatalysts for Energy-Related Applications: Oxygen Reduction, Oxygen Evolution, and Hydrogen Evolution Reactions. ACS Catalysis, 2017, 7, 7196-7225.	5.5	857
105	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
106	Anomalous Ambipolar Transport of Organic Semiconducting Crystals via Control of Molecular Packing Structures. ACS Applied Materials & Interfaces, 2017, 9, 27839-27846.	4.0	10
107	Description of ground and excited electronic states by ensemble density functional method with extended active space. Journal of Chemical Physics, 2017, 147, 064104.	1.2	27
108	Graphene and Graphene Analogs toward Optical, Electronic, Spintronic, Green-Chemical, Energy-Material, Sensing, and Medical Applications. ACS Applied Materials & Interfaces, 2017, 9, 24393-24406.	4.0	55

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109	Versatile pâ€Type Chemical Doping to Achieve Ideal Flexible Graphene Electrodes. Angewandte Chemie - International Edition, 2016, 55, 6197-6201.	7.2	78
110	Versatile pâ€Type Chemical Doping to Achieve Ideal Flexible Graphene Electrodes. Angewandte Chemie, 2016, 128, 6305-6309.	1.6	8
111	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.	2.1	39
112	Self-consistent implementation of ensemble density functional theory method for multiple strongly correlated electron pairs. Journal of Chemical Physics, 2016, 145, 244104.	1.2	23
113	Hemoglobin-carbon nanotube derived noble-metal-free Fe5C2-based catalyst for highly efficient oxygen reduction reaction. Scientific Reports, 2016, 6, 20132.	1.6	29
114	Observation of Mg-induced structural and electronic properties of graphene. Applied Physics Letters, 2016, 109, .	1.5	5
115	Halides with Fifteen Aliphatic Câ€“HÂ·Â·Â·Anion Interaction Sites. Scientific Reports, 2016, 6, 30123.	1.6	7
116	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
117	Band and bonding characteristics of N2+ ion-doped graphene. RSC Advances, 2016, 6, 84959-84964.	1.7	1
118	Oneâ€Step Synthesis of CoSâ€Doped Î²â€Co(OH)₂@Amorphous MoS₂₊_x Hybrid Catalyst Grown on Nickel Foam for Highâ€Performance Electrochemical Overall Water Splitting. Advanced Functional Materials, 2016, 26, 7386-7393.	7.8	217
119	Two-Dimensional Icy Water Clusters Between a Pair of Graphene-Like Molecules or Graphene Sheets. Journal of Physical Chemistry C, 2016, 120, 19212-19224.	1.5	1
120	Structure-mechanism-based engineering of chemical regulators targeting distinct pathological factors in Alzheimerâ€™s disease. Nature Communications, 2016, 7, 13115.	5.8	80
121	Water Splitting: One-Step Synthesis of CoS-Doped Î²-Co(OH)2 @Amorphous MoS2+ x Hybrid Catalyst Grown on Nickel Foam for High-Performance Electrochemical Overall Water Splitting (Adv. Funct.) Tj ETQq1 1 0.784314 rgBT /Overlock	4.3	
122	Halogenâ‹¯Ï€ Interactions between Benzene and X2/CX4 (X = Cl, Br): Assessment of Various Density Functionals with Respect to CCSD(T). Journal of Physical Chemistry A, 2016, 120, 9305-9314.	1.1	32
123	Electron Transport in Graphene Nanoribbon Field-Effect Transistor under Bias and Gate Voltages: Isochemical Potential Approach. Journal of Physical Chemistry Letters, 2016, 7, 2478-2482.	2.1	33
124	Covalent versus Charge Transfer Modification of Graphene/Carbon-Nanotubes with Vitamin B1: Co/N/Sâ€“C Catalyst toward Excellent Oxygen Reduction. ACS Applied Materials & Interfaces, 2016, 8, 16045-16052.	4.0	31
125	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.	1.7	13
126	Effects of an electric field on interaction of aromatic systems. Journal of Computational Chemistry, 2016, 37, 971-975.	1.5	7

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127	Using the GVB Ansatz to develop ensemble DFT method for describing multiple strongly correlated electron pairs. Physical Chemistry Chemical Physics, 2016, 18, 21040-21050.	1.3	22
128	Functional molecules and materials by Ï€â€•interaction based quantum theoretical design. International Journal of Quantum Chemistry, 2016, 116, 622-633.	1.0	29
129	Antimony(III) Sulfide Thin Films as a Photoanode Material in Photocatalytic Water Splitting. ACS Applied Materials & Interfaces, 2016, 8, 8445-8451.	4.0	73
130	Why Is MP2-Water â€œCoolerâ€•and â€œDenserâ€•than DFT-Water?. Journal of Physical Chemistry Letters, 2016, 7, 680-684.	2.1	47
131	Violation of DNA neighbor exclusion principle in RNA recognition. Chemical Science, 2016, 7, 3581-3588.	3.7	17
132	Cyanoacetic acid tethered thiophene for well-matched LUMO level in Ru(II)-terpyridine dye sensitized solar cells. Dyes and Pigments, 2016, 126, 270-278.	2.0	10
133	Engineered Carbon-Nanomaterial-Based Electrochemical Sensors for Biomolecules. ACS Nano, 2016, 10, 46-80.	7.3	433
134	Drift-induced modifications to the dynamical polarization of graphene. Physical Review B, 2015, 92, .	1.1	31
135	Hydrogenation-induced atomic stripes on the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>2</mml:mn><mml:mi>H</mml:mi></mml:mrow><mml:mn mathvariant="normal">MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>surface. Physical Review B, 2015, 92, .	1.1	32
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	Intriguing Electrostatic Potential of CO: Negative Bond-ends and Positive Bond-cylindrical-surface. Scientific Reports, 2015, 5, 16307.	1.6	29
138	Turnâ€•On Ratiometric Fluorescent Probe for Selective Discrimination of Cr³⁺ from Fe³⁺ in Aqueous Media for Living Cell Imaging. Chemistry - A European Journal, 2015, 21, 16349-16353.	1.7	22
139	Surface-Effect-Induced Optical Bandgap Shrinkage in GaN Nanotubes. Nano Letters, 2015, 15, 4472-4476.	4.5	21
140	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, 14156-14161.	3.3	27
141	Proximity Effect Induced Electronic Properties of Graphene on Bi₂Te₂Se. ACS Nano, 2015, 9, 10861-10866.	7.3	36
142	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, 6423-6432.	1.3	33
143	Controllable nâ€•Type Doping on CVDâ€•Grown Singleâ€•and Doubleâ€•Layer Graphene Mixture. Advanced Materials, 2015, 27, 1619-1623.	11.1	43
144	Triazine-Based Microporous Polymers for Selective Adsorption of CO₂. Journal of Physical Chemistry C, 2015, 119, 5395-5402.	1.5	76

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145	A Facile Route for Patterned Growth of Metalâ€“Insulator Carbon Lateral Junction through One-Pot Synthesis. ACS Nano, 2015, 9, 8352-8360.	7.3	8
146	Graphene Edges and Beyond: Temperature-Driven Structures and Electromagnetic Properties. ACS Nano, 2015, 9, 4669-4674.	7.3	31
147	Geometrical and Electronic Characteristics of Au_nO₂^{â€“} (n = 2â€“7). Journal of Physical Chemistry C, 2015, 119, 14383-14391.	1.5	13
148	Highly selective CO₂ adsorption performance of carbazole based microporous polymers. RSC Advances, 2015, 5, 41745-41750.	1.7	13
149	Interactions of CO₂with various functional molecules. Physical Chemistry Chemical Physics, 2015, 17, 10925-10933.	1.3	106
150	Tailoring Electronic and Magnetic Properties of MoS₂ Nanotubes. Journal of Physical Chemistry C, 2015, 119, 6405-6413.	1.5	40
151	Clean Transfer of Wafer-Scale Graphene via Liquid Phase Removal of Polycyclic Aromatic Hydrocarbons. ACS Nano, 2015, 9, 4726-4733.	7.3	61
152	Activated carbon derived from waste coffee grounds for stable methane storage. Nanotechnology, 2015, 26, 385602.	1.3	49
153	Disulfuric acid dissociated by two water molecules: ab initio and density functional theory calculations. Physical Chemistry Chemical Physics, 2015, 17, 28556-28564.	1.3	2
154	Anisotropic Charge Distribution and Anisotropic van der Waals Radius Leading to Intriguing Anisotropic Noncovalent Interactions. Scientific Reports, 2015, 4, 5826.	1.6	15
155	Is the Molecular Berry Phase an Artifact of the Born-Oppenheimer Approximation?. Physical Review Letters, 2014, 113, 263004.	2.9	93
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