

# Hyungjun Kim

## List of Publications by Year in Descending Order

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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.

130 papers	6,009 citations	41 h-index	74 g-index
136 ext. papers	7,672 ext. citations	11.6 avg, IF	6.14 L-index

#	Paper	IF	Citations
130	On the importance of the electric double layer structure in aqueous electrocatalysis.. <i>Nature Communications</i> , <b>2022</b> , 13, 174	17.4	13
129	Multilayer Conductive Hybrid Nanosheets as Versatile Hybridization Matrices for Optimizing the Defect Structure, Structural Ordering, and Energy-Functionality of Nanostructured Materials. <i>Advanced Science</i> , <b>2021</b> , e2103042	13.6	3
128	Selective electrochemical reduction of nitric oxide to hydroxylamine by atomically dispersed iron catalyst. <i>Nature Communications</i> , <b>2021</b> , 12, 1856	17.4	25
127	Redirecting dynamic surface restructuring of a layered transition metal oxide catalyst for superior water oxidation. <i>Nature Catalysis</i> , <b>2021</b> , 4, 212-222	36.5	80
126	Tailoring a Dynamic Metal-Polymer Interaction to Improve Catalyst Selectivity and Longevity in Hydrogenation. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 12590-12597	3.6	
125	Tailoring a Dynamic Metal-Polymer Interaction to Improve Catalyst Selectivity and Longevity in Hydrogenation. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 12482-12489	16.4	7
124	Lattice Engineering to Simultaneously Control the Defect/Stacking Structures of Layered Double Hydroxide Nanosheets to Optimize Their Energy Functionalities. <i>ACS Nano</i> , <b>2021</b> , 15, 8306-8318	16.7	16
123	Femtosecond Quantum Dynamics of Excited-State Evolution of Halide Perovskites: Quantum Chaos of Molecular Cations. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 10676-10684	3.8	1
122	Microbially Guided Discovery and Biosynthesis of Biologically Active Natural Products. <i>ACS Synthetic Biology</i> , <b>2021</b> , 10, 1505-1519	5.7	3
121	Identification of Single-Atom Ni Site Active toward Electrochemical CO Conversion to CO. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 925-933	16.4	39
120	Dynamic Transformation of a Ag-Coordinated Supramolecular Nanostructure from a 1D Needle to a 1D Helical Tube via a 2D Ribbon Accompanying the Conversion of Complex Structures. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 3113-3123	16.4	6
119	Simultaneous Enhanced Efficiency and Stability of Perovskite Solar Cells Using Adhesive Fluorinated Polymer Interfacial Material. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2021</b> , 13, 35595-35605	9.5	8
118	Physicochemical Understanding of the Impact of Pore Environment and Species of Adsorbates on Adsorption Behaviour. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 20504-20510	16.4	2
117	Assessment and prediction of band edge locations of nitrides using a self-consistent hybrid functional. <i>Journal of Chemical Physics</i> , <b>2021</b> , 155, 024120	3.9	1
116	Reversible Ligand Exchange in Atomically Dispersed Catalysts for Modulating the Activity and Selectivity of the Oxygen Reduction Reaction. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 20528-20534	16.4	4
115	Reversible Ligand Exchange in Atomically Dispersed Catalysts for Modulating the Activity and Selectivity of the Oxygen Reduction Reaction. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 20691-20697	3.6	0
114	Water Slippage on Graphitic and Metallic Surfaces: Impact of the Surface Packing Structure and Electron Density Tail. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 11392-11400	3.8	2

113	Electrocatalysts: Synergistic Control of Structural Disorder and Surface Bonding Nature to Optimize the Functionality of Manganese Oxide as an Electrocatalyst and a Cathode for Li-O <sub>2</sub> Batteries (Small 12/2020). <i>Small</i> , <b>2020</b> , 16, 2070062	11	
112	Monolayered g-C <sub>3</sub> N <sub>4</sub> nanosheet as an emerging cationic building block for bifunctional 2D superlattice hybrid catalysts with controlled defect structures. <i>Applied Catalysis B: Environmental</i> , <b>2020</b> , 277, 119191	21.8	31
111	Effect of groundwater ions (Ca, Na, and HCO <sub>3</sub> <sup>-</sup> ) on removal of hexavalent chromium by Fe(II)-phosphate mineral. <i>Journal of Hazardous Materials</i> , <b>2020</b> , 398, 122948	12.8	10
110	Dynamic metal-polymer interaction for the design of chemoselective and long-lived hydrogenation catalysts. <i>Science Advances</i> , <b>2020</b> , 6, eabb7369	14.3	21
109	uMBD: A Materials-Ready Dispersion Correction That Uniformly Treats Metallic, Ionic, and van der Waals Bonding. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 2346-2354	16.4	21
108	Spectroscopic capture of a low-spin Mn(IV)-oxo species in Ni-MnO nanoparticles during water oxidation catalysis. <i>Nature Communications</i> , <b>2020</b> , 11, 5230	17.4	7
107	A General Strategy to Atomically Dispersed Precious Metal Catalysts for Unravelling Their Catalytic Trends for Oxygen Reduction Reaction. <i>ACS Nano</i> , <b>2020</b> , 14, 1990-2001	16.7	58
106	Activity-Stability Relationship in [email-protected] Nanoparticles for Electrocatalysis. <i>ACS Energy Letters</i> , <b>2020</b> , 5, 2827-2834	20.1	22
105	Unveiling Electrode-Electrolyte Design-Based NO Reduction for NH <sub>3</sub> Synthesis. <i>ACS Energy Letters</i> , <b>2020</b> , 5, 3647-3656	20.1	39
104	Time-resolved observation of CO <sub>2</sub> coupling intermediates on Cu electrodes for selective electrochemical CO <sub>2</sub> reduction. <i>Energy and Environmental Science</i> , <b>2020</b> , 13, 4301-4311	35.4	63
103	High-performance p-channel transistors with transparent Zn doped-CuI. <i>Nature Communications</i> , <b>2020</b> , 11, 4309	17.4	38
102	Thermal Transformation of Molecular Ni <sub>2</sub> +Ni <sub>4</sub> Sites for Enhanced CO <sub>2</sub> Electroreduction Activity. <i>ACS Catalysis</i> , <b>2020</b> , 10, 10920-10931	13.1	32
101	Intermetallic PtCu Nanoframes as Efficient Oxygen Reduction Electrocatalysts. <i>Nano Letters</i> , <b>2020</b> , 20, 7413-7421	11.5	46
100	FeNi <sub>2</sub> -P Alloy Nanocatalysts with Electron-Deficient Phosphorus Enhancing the Hydrogen Evolution Reaction in Acidic Media. <i>ACS Catalysis</i> , <b>2020</b> , 10, 11665-11673	13.1	16
99	Operando Stability of Platinum Electrocatalysts in Ammonia Oxidation Reactions. <i>ACS Catalysis</i> , <b>2020</b> , 10, 11674-11684	13.1	10
98	Electric Field Mediated Selectivity Switching of Electrochemical CO <sub>2</sub> Reduction from Formate to CO on Carbon Supported Sn. <i>ACS Energy Letters</i> , <b>2020</b> , 5, 2987-2994	20.1	20
97	Synergistic Control of Structural Disorder and Surface Bonding Nature to Optimize the Functionality of Manganese Oxide as an Electrocatalyst and a Cathode for Li-O Batteries. <i>Small</i> , <b>2020</b> , 16, e1903265	11	17
96	Thermodynamics of Multicomponent Perovskites: A Guide to Highly Efficient and Stable Solar Cell Materials. <i>Chemistry of Materials</i> , <b>2020</b> , 32, 4265-4272	9.6	13

95	Electronic Structure and Band Alignments of Various Phases of Titania Using the Self-Consistent Hybrid Density Functional and DFT+ Methods. <i>Frontiers in Chemistry</i> , <b>2019</b> , 7, 47	5	7
94	Understanding the relative efficacies and versatile roles of 2D conductive nanosheets in hybrid-type photocatalyst. <i>Applied Catalysis B: Environmental</i> , <b>2019</b> , 257, 117875	21.8	14
93	Ligand-Controlled Direct Hydroformylation of Trisubstituted Olefins. <i>Organic Letters</i> , <b>2019</b> , 21, 5789-5792	9.2	7
92	Experimental and Density Functional Theory Corroborated Optimization of Durable Metal Embedded Carbon Nanofiber for Oxygen Electrocatalysis. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 3109-3114	6.4	11
91	Ultrafast charge transfer coupled with lattice phonons in two-dimensional covalent organic frameworks. <i>Nature Communications</i> , <b>2019</b> , 10, 1873	17.4	55
90	Reversible and cooperative photoactivation of single-atom Cu/TiO photocatalysts. <i>Nature Materials</i> , <b>2019</b> , 18, 620-626	27	275
89	Self-Assembly of a Peptide Foldamer: The Role of the Surfactant in Three-Dimensional Shape Selection. <i>ChemPlusChem</i> , <b>2019</b> , 84, 481-487	2.8	7
88	Light Emission Enhancement by Tuning the Structural Phase of APbBr (A = CHNH, Cs) Perovskites. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 2135-2142	6.4	9
87	Enthalpy-Entropy Interplay in Stacking Interaction of Benzene Dimer in Water. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 1538-1545	6.4	10
86	Metal-Oxide Interfaces for Selective Electrochemical CO Coupling Reactions. <i>ACS Energy Letters</i> , <b>2019</b> , 4, 2241-2248	20.1	34
85	Porous Metal-Organic Framework CUK-1 for Adsorption Heat Allocation toward Green Applications of Natural Refrigerant Water. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 25778-25789	9.5	23
84	Structure, Dynamics, and Wettability of Water at Metal Interfaces. <i>Scientific Reports</i> , <b>2019</b> , 9, 14805	4.9	21
83	Selectivity Modulated by Surface Ligands on Cu <sub>2</sub> O/TiO <sub>2</sub> Catalysts for Gas-Phase Photocatalytic Reduction of Carbon Dioxide. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 29184-29191	3.8	14
82	Activity Origin and Multifunctionality of Pt-Based Intermetallic Nanostructures for Efficient Electrocatalysis. <i>ACS Catalysis</i> , <b>2019</b> , 9, 11242-11254	13.1	56
81	Probing Surface Chemistry at an Atomic Level: Decomposition of 1-Propanethiol on GaP(001) (2 × 4) Investigated by STM, XPS, and DFT. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 2964-2972	3.8	
80	Cluster Expansion Method for Simulating Realistic Size of Nanoparticle Catalysts with an Application in CO <sub>2</sub> Electroreduction. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 9245-9254	3.8	12
79	Polymeric Carbon Nitride with Localized Aluminum Coordination Sites as a Durable and Efficient Photocatalyst for Visible Light Utilization. <i>ACS Catalysis</i> , <b>2018</b> , 8, 4241-4256	13.1	84
78	Electrochemical Evidence for Two Sub-families of FeN <sub>x</sub> C <sub>y</sub> Moieties with Concentration-Dependent Cyanide Poisoning. <i>ChemElectroChem</i> , <b>2018</b> , 5, 1880-1885	4.3	18

77	Benchmarking several van der Waals dispersion approaches for the description of intermolecular interactions. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 064112	3.9	33
76	Mixed Valence Perovskite Cs Au I : A Potential Material for Thin-Film Pb-Free Photovoltaic Cells with Ultrahigh Efficiency. <i>Advanced Materials</i> , <b>2018</b> , 30, e1707001	24	54
75	Insight into the Microenvironments of the Metal/Ionic Liquid Interface during Electrochemical CO <sub>2</sub> Reduction. <i>ACS Catalysis</i> , <b>2018</b> , 8, 2420-2427	13.1	52
74	Solid Electrolyte Layers by Solution Deposition. <i>Advanced Materials Interfaces</i> , <b>2018</b> , 5, 1701328	4.6	35
73	Exfoliated 2D Lepidocrocite Titanium Oxide Nanosheets for High Sulfur Content Cathodes with Highly Stable Li/S Battery Performance. <i>ACS Energy Letters</i> , <b>2018</b> , 3, 412-419	20.1	78
72	First-Principles Studies on Twinnability of Magnesium Alloys: Effects of Yttrium and Lithium on (left( {10\bar{1}1} right)left[ {1\bar{1}02} right]) Compression Twinning Deformation Processes. <i>Metals and Materials International</i> , <b>2018</b> , 24, 720-729	2.4	5
71	Ga-Doped Pt-Ni Octahedral Nanoparticles as a Highly Active and Durable Electrocatalyst for Oxygen Reduction Reaction. <i>Nano Letters</i> , <b>2018</b> , 18, 2450-2458	11.5	82
70	Multiscale Simulation Method for Quantitative Prediction of Surface Wettability at the Atomistic Level. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 1750-1758	6.4	17
69	Bifunctional 2D Superlattice Electrocatalysts of Layered Double Hydroxide/Transition Metal Dichalcogenide Active for Overall Water Splitting. <i>ACS Energy Letters</i> , <b>2018</b> , 3, 952-960	20.1	89
68	A rational method to kinetically control the rate-determining step to explore efficient electrocatalysts for the oxygen evolution reaction. <i>NPG Asia Materials</i> , <b>2018</b> , 10, 659-669	10.3	35
67	Heterolayered 2D nanohybrids of uniformly stacked transition metal dichalcogenide/transition metal oxide monolayers with improved energy-related functionalities. <i>Journal of Materials Chemistry A</i> , <b>2018</b> , 6, 15237-15244	13	25
66	A hydro/oxo-phobic top hole-selective layer for efficient and stable colloidal quantum dot solar cells. <i>Energy and Environmental Science</i> , <b>2018</b> , 11, 2078-2084	35.4	31
65	Molecular Identification of Cr(VI) Removal Mechanism on Vivianite Surface. <i>Environmental Science &amp; Technology</i> , <b>2018</b> , 52, 10647-10656	10.3	30
64	The Achilles'Heel of iron-based catalysts during oxygen reduction in an acidic medium. <i>Energy and Environmental Science</i> , <b>2018</b> , 11, 3176-3182	35.4	208
63	Hydration Thermodynamics of Non-Polar Aromatic Hydrocarbons: Comparison of Implicit and Explicit Solvation Models. <i>Molecules</i> , <b>2018</b> , 23,	4.8	8
62	Roles of SnX (X = F, Cl, Br) Additives in Tin-Based Halide Perovskites toward Highly Efficient and Stable Lead-Free Perovskite Solar Cells. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 6024-6031	6.4	88
61	Superior role of MXene nanosheet as hybridization matrix over graphene in enhancing interfacial electronic coupling and functionalities of metal oxide. <i>Nano Energy</i> , <b>2018</b> , 53, 841-848	17.1	27
60	Solid Electrolyte: Solid Electrolyte Layers by Solution Deposition (Adv. Mater. Interfaces 8/2018). <i>Advanced Materials Interfaces</i> , <b>2018</b> , 5, 1870035	4.6	1

59	PMnO <sub>2</sub> Nanowire-Anchored Highly Oxidized Cluster as a Catalyst for Li-O <sub>2</sub> Batteries: Superior Electrocatalytic Activity and High Functionality. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 16216-16221	3.6	4
58	PMnO Nanowire-Anchored Highly Oxidized Cluster as a Catalyst for Li-O Batteries: Superior Electrocatalytic Activity and High Functionality. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 15984-15989	16.4	54
57	Carbon Monoxide as a Promoter of Atomically Dispersed Platinum Catalyst in Electrochemical Hydrogen Evolution Reaction. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 16198-16205	16.4	55
56	Impacts of cation ordering on bandgap dispersion of double perovskites. <i>APL Materials</i> , <b>2018</b> , 6, 084903	5.7	10
55	Polymorphic Phase Control Mechanism of Organic-Inorganic Hybrid Perovskite Engineered by Dual-Site Alloying. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 9508-9515	3.8	14
54	High-efficiency and high-power rechargeable lithium-sulfur dioxide batteries exploiting conventional carbonate-based electrolytes. <i>Nature Communications</i> , <b>2017</b> , 8, 14989	17.4	31
53	Facile CO <sub>2</sub> Electro-Reduction to Formate via Oxygen Bidentate Intermediate Stabilized by High-Index Planes of Bi Dendrite Catalyst. <i>ACS Catalysis</i> , <b>2017</b> , 7, 5071-5077	13.1	182
52	Synergistic interaction of Re complex and amine functionalized multiple ligands in metal-organic frameworks for conversion of carbon dioxide. <i>Scientific Reports</i> , <b>2017</b> , 7, 612	4.9	47
51	Nitrate reduction on the surface of bimetallic catalysts supported by nano-crystalline beta-zeolite (NBeta). <i>Green Chemistry</i> , <b>2017</b> , 19, 853-866	10	26
50	Insight into Electrochemical CO <sub>2</sub> Reduction on Surface-Molecule-Mediated Ag Nanoparticles. <i>ACS Catalysis</i> , <b>2017</b> , 7, 779-785	13.1	151
49	Band Gap Engineering of Cs <sub>3</sub> Bi <sub>2</sub> I <sub>9</sub> Perovskites with Trivalent Atoms Using a Dual Metal Cation. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 969-974	3.8	31
48	Distorted Carbon Nitride Structure with Substituted Benzene Moieties for Enhanced Visible Light Photocatalytic Activities. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2017</b> , 9, 40360-40368	9.5	50
47	Highly selective adsorption of p-xylene over other C aromatic hydrocarbons by Co-CUK-1: a combined experimental and theoretical assessment. <i>Dalton Transactions</i> , <b>2017</b> , 46, 16096-16101	4.3	14
46	New Features and Uncovered Benefits of Polycrystalline Magnetite as Reusable Catalyst in Reductive Chemical Conversion. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 25195-25205	3.8	15
45	The Mechanism of Room-Temperature Ionic-Liquid-Based Electrochemical CO <sub>2</sub> Reduction: A Review. <i>Molecules</i> , <b>2017</b> , 22,	4.8	42
44	Transfer and Dynamic Inversion of Coassembled Supramolecular Chirality through 2D-Sheet to Rolled-Up Tubular Structure. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 17711-17714	16.4	43
43	Zinc-Phosphorus Complex Working as an Atomic Valve for Colloidal Growth of Monodisperse Indium Phosphide Quantum Dots. <i>Chemistry of Materials</i> , <b>2017</b> , 29, 6346-6355	9.6	39
42	A Seamless Grid-Based Interface for Mean-Field QM/MM Coupled with Efficient Solvation Free Energy Calculations. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 5088-5099	6.4	22

41	Tuning selectivity of electrochemical reactions by atomically dispersed platinum catalyst. <i>Nature Communications</i> , <b>2016</b> , 7, 10922	17.4	509
40	Tuned Chemical Bonding Ability of Au at Grain Boundaries for Enhanced Electrochemical CO <sub>2</sub> Reduction. <i>ACS Catalysis</i> , <b>2016</b> , 6, 4443-4448	13.1	78
39	A mechanistic model for hydrogen activation, spillover, and its chemical reaction in a zeolite-encapsulated Pt catalyst. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 7035-41	3.6	24
38	Effect of NaBH <sub>4</sub> on properties of nanoscale zero-valent iron and its catalytic activity for reduction of p -nitrophenol. <i>Applied Catalysis B: Environmental</i> , <b>2016</b> , 182, 541-549	21.8	167
37	A Conductive Hybridization Matrix of RuO <sub>2</sub> Two-Dimensional Nanosheets: A Hybrid-Type Photocatalyst. <i>Angewandte Chemie - International Edition</i> , <b>2016</b> , 55, 8546-50	16.4	41
36	Laser-induced phase separation of silicon carbide. <i>Nature Communications</i> , <b>2016</b> , 7, 13562	17.4	47
35	Recent development of atom-pairwise van der waals corrections for density functional theory: From molecules to solids. <i>International Journal of Quantum Chemistry</i> , <b>2016</b> , 116, 598-607	2.1	15
34	Exfoliated Metal Oxide Nanosheets as Effective and Applicable Substrates for Atomically Dispersed Metal Nanoparticles with Tailorable Functionalities. <i>Advanced Materials Interfaces</i> , <b>2016</b> , 3, 1600661	4.6	3
33	2D Covalent Metals: A New Materials Domain of Electrochemical CO Conversion with Broken Scaling Relationship. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 4124-4129	6.4	45
32	Failure of Density Functional Dispersion Correction in Metallic Systems and Its Possible Solution Using a Modified Many-Body Dispersion Correction. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 3278-834	6.4	10
31	Highly Efficient, Selective, and Stable CO <sub>2</sub> Electroreduction on a Hexagonal Zn Catalyst. <i>Angewandte Chemie</i> , <b>2016</b> , 128, 9443-9446	3.6	41
30	Highly Efficient, Selective, and Stable CO <sub>2</sub> Electroreduction on a Hexagonal Zn Catalyst. <i>Angewandte Chemie - International Edition</i> , <b>2016</b> , 55, 9297-300	16.4	227
29	Probing Distinct Fullerene Formation Processes from Carbon Precursors of Different Sizes and Structures. <i>Analytical Chemistry</i> , <b>2016</b> , 88, 8232-8	7.8	6
28	Hydrogen Spillover in Encapsulated Metal Catalysts: New Opportunities for Designing Advanced Hydroprocessing Catalysts. <i>ChemCatChem</i> , <b>2015</b> , 7, 1048-1057	5.2	35
27	Theoretical and experimental studies of the dechlorination mechanism of carbon tetrachloride on a vivianite ferrous phosphate surface. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 5714-22	2.8	12
26	Induction and control of supramolecular chirality by light in self-assembled helical nanostructures. <i>Nature Communications</i> , <b>2015</b> , 6, 6959	17.4	128
25	Magnetotactic molecular architectures from self-assembly of $\beta$ -peptide foldamers. <i>Nature Communications</i> , <b>2015</b> , 6, 8747	17.4	50
24	Achieving Selective and Efficient Electrocatalytic Activity for CO <sub>2</sub> Reduction Using Immobilized Silver Nanoparticles. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 13844-50	16.4	437

23	Phase Tuning of Nanostructured Gallium Oxide via Hybridization with Reduced Graphene Oxide for Superior Anode Performance in Li-Ion Battery: An Experimental and Theoretical Study. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2015</b> , 7, 18679-88	9.5	41
22	Prediction of the reduction potential of tris(2,2Sbipyridinyl)iron(III/II) derivatives. <i>Journal of Computational Chemistry</i> , <b>2015</b> , 36, 33-41	3.5	8
21	Nitrite reduction mechanism on a Pd surface. <i>Environmental Science &amp; Technology</i> , <b>2014</b> , 48, 12768-74	10.3	105
20	Selective Dissociation of Dihydrogen over Dioxygen on a Hindered Platinum Surface for the Direct Synthesis of Hydrogen Peroxide. <i>ChemCatChem</i> , <b>2014</b> , 6, 2836-2842	5.2	18
19	Maximizing the catalytic function of hydrogen spillover in platinum-encapsulated aluminosilicates with controlled nanostructures. <i>Nature Communications</i> , <b>2014</b> , 5, 3370	17.4	117
18	Embedding covalency into metal catalysts for efficient electrochemical conversion of CO <sub>2</sub> . <i>Journal of the American Chemical Society</i> , <b>2014</b> , 136, 11355-61	16.4	157
17	Effect of marine environmental factors on the phase equilibrium of CO <sub>2</sub> hydrate. <i>International Journal of Greenhouse Gas Control</i> , <b>2014</b> , 20, 285-292	4.2	23
16	Long-range electron transfer over graphene-based catalyst for high-performing oxygen reduction reactions: importance of size, N-doping, and metallic impurities. <i>Journal of the American Chemical Society</i> , <b>2014</b> , 136, 9070-7	16.4	256
15	First-Principles Design of Hydrogen Dissociation Catalysts Based on Isoelectronic Metal Solid Solutions. <i>Journal of Physical Chemistry Letters</i> , <b>2014</b> , 5, 1819-24	6.4	21
14	Rapid Dye Regeneration Mechanism of Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry Letters</i> , <b>2014</b> , 5, 4285-90	6.4	19
13	A protocol to evaluate one electron redox potential for iron complexes. <i>Journal of Computational Chemistry</i> , <b>2013</b> , 34, 2233-41	3.5	26
12	Inner-sphere electron-transfer single iodide mechanism for dye regeneration in dye-sensitized solar cells. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 2431-4	16.4	26
11	DFT Study of Water Adsorption and Decomposition on a Ga-Rich GaP(001)(2 $\times$ 8) Surface. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 17604-17612	3.8	27
10	Turning On MLCT Phosphorescence of Iridium(III)Borane Conjugates upon Fluoride Binding. <i>Organometallics</i> , <b>2012</b> , 31, 31-34	3.8	40
9	The Role of Confined Water in Ionic Liquid Electrolytes for Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry Letters</i> , <b>2012</b> , 3, 556-9	6.4	28
8	Anisotropic Shock Sensitivity of Cyclotrimethylene Trinitramine (RDX) from Compress-and-Shear Reactive Dynamics. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 10198-10206	3.8	64
7	Universal Correction of Density Functional Theory to Include London Dispersion (up to Lr, Element 103). <i>Journal of Physical Chemistry Letters</i> , <b>2012</b> , 3, 360-3	6.4	41
6	High-temperature high-pressure phases of lithium from electron force field (eFF) quantum electron dynamics simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2011</b> , 108, 15101-5	11.5	20

5	Wall-mediated self-diffusion in slit and cylindrical pores. <i>Physical Review E</i> , <b>2008</b> , 77, 031202	2.4	8
4	DYNAMICS OF SIMPLE FLUIDS CONFINED IN CYLINDRICAL PORE: EFFECT OF PORE SIZE. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2005</b> , 04, 305-315	1.8	6
3	Density functional theory in classical explicit solvents: Mean-field QM / MM method for simulating solid-liquid interfaces. <i>Bulletin of the Korean Chemical Society</i> ,	1.2	1
2	Electronic interaction between transition metal single-atoms and anatase TiO <sub>2</sub> boosts CO <sub>2</sub> photoreduction with H <sub>2</sub> O. <i>Energy and Environmental Science</i> ,	35.4	14
1	Triphasic Metal Oxide Photocatalyst for Reaction Site-Specific Production of Hydrogen Peroxide from Oxygen Reduction and Water Oxidation. <i>Advanced Energy Materials</i> , 2104052	21.8	1