Hyungjun Kim

List of Publications by Year
in descending order

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Version: 2024-02-01

135 papers	9,500 citations	38742 50 h-index	40979 93 g-index

136 all docs	136 docs citations	136 times ranked	12185 citing authors

#	Article	IF	Citations
1	Electronic interaction between transition metal single-atoms and anatase TiO₂ boosts CO₂ photoreduction with H₂O. Energy and Environmental Science, 2022, 15, 601-609.	30.8	88
2	Multilayer Conductive Hybrid Nanosheets as Versatile Hybridization Matrices for Optimizing the Defect Structure, Structural Ordering, and Energyâ€Functionality of Nanostructured Materials. Advanced Science, 2022, 9, e2103042.	11.2	19
3	On the importance of the electric double layer structure in aqueous electrocatalysis. Nature Communications, 2022, 13, 174.	12.8	92
4	Density functional theory in classical explicit solvents: Meanâ€field <scp>QM</scp>/<scp>MM</scp> method for simulating solidâ€“liquid interfaces. Bulletin of the Korean Chemical Society, 2022, 43, 476-483.	1.9	7
5	Interface rich CuO/Al₂CuO₄ surface for selective ethylene production from electrochemical CO₂ conversion. Energy and Environmental Science, 2022, 15, 2397-2409.	30.8	54
6	Triphasic Metal Oxide Photocatalyst for Reaction Siteâ€Specific Production of Hydrogen Peroxide from Oxygen Reduction and Water Oxidation. Advanced Energy Materials, 2022, 12, .	19.5	17
7	Enhanced Light Emission through Symmetry Engineering of Halide Perovskites. Journal of the American Chemical Society, 2022, 144, 297-305.	13.7	5
8	Identification of Single-Atom Ni Site Active toward Electrochemical CO₂ Conversion to CO. Journal of the American Chemical Society, 2021, 143, 925-933.	13.7	107
9	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. Journal of the American Chemical Society, 2021, 143, 3113-3123.	13.7	24
10	Selective electrochemical reduction of nitric oxide to hydroxylamine by atomically dispersed iron catalyst. Nature Communications, 2021, 12, 1856.	12.8	106
11	Redirecting dynamic surface restructuring of a layered transition metal oxide catalyst for superior water oxidation. Nature Catalysis, 2021, 4, 212-222.	34.4	266
12	Tailoring a Dynamic Metalâ€“Polymer Interaction to Improve Catalyst Selectivity and Longevity in Hydrogenation. Angewandte Chemie, 2021, 133, 12590-12597.	2.0	0
13	Tailoring a Dynamic Metalâ€“Polymer Interaction to Improve Catalyst Selectivity and Longevity in Hydrogenation. Angewandte Chemie - International Edition, 2021, 60, 12482-12489.	13.8	19
14	Lattice Engineering to Simultaneously Control the Defect/Stacking Structures of Layered Double Hydroxide Nanosheets to Optimize Their Energy Functionalities. ACS Nano, 2021, 15, 8306-8318.	14.6	49
15	Femtosecond Quantum Dynamics of Excited-State Evolution of Halide Perovskites: Quantum Chaos of Molecular Cations. Journal of Physical Chemistry C, 2021, 125, 10676-10684.	3.1	1
16	Microbially Guided Discovery and Biosynthesis of Biologically Active Natural Products. ACS Synthetic Biology, 2021, 10, 1505-1519.	3.8	11
17	Simultaneous Enhanced Efficiency and Stability of Perovskite Solar Cells Using Adhesive Fluorinated Polymer Interfacial Material. ACS Applied Materials & Interfaces, 2021, 13, 35595-35605.	8.0	20
18	Physicochemical Understanding of the Impact of Pore Environment and Species of Adsorbates on Adsorption Behaviour. Angewandte Chemie - International Edition, 2021, 60, 20504-20510.	13.8	8

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19	Assessment and prediction of band edge locations of nitrides using a self-consistent hybrid functional. Journal of Chemical Physics, 2021, 155, 024120.	3.0	1
20	Reversible Ligand Exchange in Atomically Dispersed Catalysts for Modulating the Activity and Selectivity of the Oxygen Reduction Reaction. Angewandte Chemie - International Edition, 2021, 60, 20528-20534.	13.8	27
21	Reversible Ligand Exchange in Atomically Dispersed Catalysts for Modulating the Activity and Selectivity of the Oxygen Reduction Reaction. Angewandte Chemie, 2021, 133, 20691-20697.	2.0	3
22	In Situ Mapping and Local Negative Uptake Behavior of Adsorbates in Individual Pores of Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2021, 143, 20747-20757.	13.7	5
23	Synergistic Control of Structural Disorder and Surface Bonding Nature to Optimize the Functionality of Manganese Oxide as an Electrocatalyst and a Cathode for Liâ€“O 2 Batteries. Small, 2020, 16, 1903265.	10.0	26
24	uMBD: A Materials-Ready Dispersion Correction That Uniformly Treats Metallic, Ionic, and van der Waals Bonding. Journal of the American Chemical Society, 2020, 142, 2346-2354.	13.7	29
25	Spectroscopic capture of a low-spin Mn(IV)-oxo species in Niâ€“Mn3O4 nanoparticles during water oxidation catalysis. Nature Communications, 2020, 11, 5230.	12.8	21
26	A General Strategy to Atomically Dispersed Precious Metal Catalysts for Unravelling Their Catalytic Trends for Oxygen Reduction Reaction. ACS Nano, 2020, 14, 1990-2001.	14.6	116
27	Activityâ€“Stability Relationship in Au@Pt Nanoparticles for Electrocatalysis. ACS Energy Letters, 2020, 5, 2827-2834.	17.4	49
28	Unveiling Electrodeâ€“Electrolyte Design-Based NO Reduction for NH₃ Synthesis. ACS Energy Letters, 2020, 5, 3647-3656.	17.4	97
29	Time-resolved observation of Câ€“C coupling intermediates on Cu electrodes for selective electrochemical CO₂ reduction. Energy and Environmental Science, 2020, 13, 4301-4311.	30.8	197
30	High-performance p-channel transistors with transparent Zn doped-CuI. Nature Communications, 2020, 11, 4309.	12.8	94
31	Thermal Transformation of Molecular Ni²⁺â€“N₄ Sites for Enhanced CO₂ Electroreduction Activity. ACS Catalysis, 2020, 10, 10920-10931.	11.2	81
32	Intermetallic PtCu Nanoframes as Efficient Oxygen Reduction Electrocatalysts. Nano Letters, 2020, 20, 7413-7421.	9.1	109
33	Fe_xNi_{2â€“x}P Alloy Nanocatalysts with Electron-Deficient Phosphorus Enhancing the Hydrogen Evolution Reaction in Acidic Media. ACS Catalysis, 2020, 10, 11665-11673.	11.2	41
34	Operando Stability of Platinum Electrocatalysts in Ammonia Oxidation Reactions. ACS Catalysis, 2020, 10, 11674-11684.	11.2	36
35	Electric Field Mediated Selectivity Switching of Electrochemical CO₂ Reduction from Formate to CO on Carbon Supported Sn. ACS Energy Letters, 2020, 5, 2987-2994.	17.4	41
36	Water Slippage on Graphitic and Metallic Surfaces: Impact of the Surface Packing Structure and Electron Density Tail. Journal of Physical Chemistry C, 2020, 124, 11392-11400.	3.1	6

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37	Electrocatalysts: Synergistic Control of Structural Disorder and Surface Bonding Nature to Optimize the Functionality of Manganese Oxide as an Electrocatalyst and a Cathode for Liâ€“O₂ Batteries (Small 12/2020). Small, 2020, 16, 2070062.	10.0	1
38	Monolayered g-C3N4 nanosheet as an emerging cationic building block for bifunctional 2D superlattice hybrid catalysts with controlled defect structures. Applied Catalysis B: Environmental, 2020, 277, 119191.	20.2	56
39	Effect of groundwater ions (Ca2+, Na+, and HCO3â¯) on removal of hexavalent chromium by Fe(II)-phosphate mineral. Journal of Hazardous Materials, 2020, 398, 122948.	12.4	15
40	Dynamic metal-polymer interaction for the design of chemoselective and long-lived hydrogenation catalysts. Science Advances, 2020, 6, eabb7369.	10.3	53
41	Thermodynamics of Multicomponent Perovskites: A Guide to Highly Efficient and Stable Solar Cell Materials. Chemistry of Materials, 2020, 32, 4265-4272.	6.7	26
42	Metalâ€“Oxide Interfaces for Selective Electrochemical Câ€“C Coupling Reactions. ACS Energy Letters, 2019, 4, 2241-2248.	17.4	62
43	Porous Metalâ€“Organic Framework CUK-1 for Adsorption Heat Allocation toward Green Applications of Natural Refrigerant Water. ACS Applied Materials & Interfaces, 2019, 11, 25778-25789.	8.0	45
44	Structure, Dynamics, and Wettability of Water at Metal Interfaces. Scientific Reports, 2019, 9, 14805.	3.3	38
45	Selectivity Modulated by Surface Ligands on Cu₂O/TiO₂ Catalysts for Gas-Phase Photocatalytic Reduction of Carbon Dioxide. Journal of Physical Chemistry C, 2019, 123, 29184-29191.	3.1	27
46	Activity Origin and Multifunctionality of Pt-Based Intermetallic Nanostructures for Efficient Electrocatalysis. ACS Catalysis, 2019, 9, 11242-11254.	11.2	96
47	Electronic Structure and Band Alignments of Various Phases of Titania Using the Self-Consistent Hybrid Density Functional and DFT+U Methods. Frontiers in Chemistry, 2019, 7, 47.	3.6	12
48	Understanding the relative efficacies and versatile roles of 2D conductive nanosheets in hybrid-type photocatalyst. Applied Catalysis B: Environmental, 2019, 257, 117875.	20.2	19
49	Ligand-Controlled Direct Hydroformylation of Trisubstituted Olefins. Organic Letters, 2019, 21, 5789-5792.	4.6	17
50	Experimental and Density Functional Theory Corroborated Optimization of Durable Metal Embedded Carbon Nanofiber for Oxygen Electrocatalysis. Journal of Physical Chemistry Letters, 2019, 10, 3109-3114.	4.6	16
51	Ultrafast charge transfer coupled with lattice phonons in two-dimensional covalent organic frameworks. Nature Communications, 2019, 10, 1873.	12.8	93
52	Reversible and cooperative photoactivation of single-atom Cu/TiO2 photocatalysts. Nature Materials, 2019, 18, 620-626.	27.5	501
53	Selfâ€Assembly of a Î²â€Peptide Foldamer: The Role of the Surfactant in Threeâ€Dimensional Shape Selection. ChemPlusChem, 2019, 84, 481-487.	2.8	10
54	Light Emission Enhancement by Tuning the Structural Phase of APbBr₃ (A =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 67 Td (C 2135-2142.	4.6	12

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55	Enthalpyâ€“Entropy Interplay in Ï€-Stacking Interaction of Benzene Dimer in Water. Journal of Chemical Theory and Computation, 2019, 15, 1538-1545.	5.3	16
56	Probing Surface Chemistry at an Atomic Level: Decomposition of 1-Propanethiol on GaP(001) (2 Ã— 4) Investigated by STM, XPS, and DFT. Journal of Physical Chemistry C, 2019, 123, 2964-2972.	3.1	0
57	Cluster Expansion Method for Simulating Realistic Size of Nanoparticle Catalysts with an Application in CO₂ Electroreduction. Journal of Physical Chemistry C, 2018, 122, 9245-9254.	3.1	17
58	Polymeric Carbon Nitride with Localized Aluminum Coordination Sites as a Durable and Efficient Photocatalyst for Visible Light Utilization. ACS Catalysis, 2018, 8, 4241-4256.	11.2	118
59	Electrochemical Evidence for Two Subâ€families of FeN_xC_y Moieties with Concentrationâ€Dependent Cyanide Poisoning. ChemElectroChem, 2018, 5, 1880-1885.	3.4	24
60	Benchmarking several van der Waals dispersion approaches for the description of intermolecular interactions. Journal of Chemical Physics, 2018, 148, 064112.	3.0	37
61	Mixed Valence Perovskite Cs₂Au₂I₆: A Potential Material for Thinâ€Film Pbâ€Free Photovoltaic Cells with Ultrahigh Efficiency. Advanced Materials, 2018, 30, e1707001.	21.0	79
62	Insight into the Microenvironments of the Metalâ€“Ionic Liquid Interface during Electrochemical CO₂ Reduction. ACS Catalysis, 2018, 8, 2420-2427.	11.2	77
63	Solid Electrolyte Layers by Solution Deposition. Advanced Materials Interfaces, 2018, 5, 1701328.	3.7	42
64	Exfoliated 2D Lepidocrocite Titanium Oxide Nanosheets for High Sulfur Content Cathodes with Highly Stable Liâ€“S Battery Performance. ACS Energy Letters, 2018, 3, 412-419.	17.4	90
65	First-Principles Studies on Twinnability of Magnesium Alloys: Effects of Yttrium and Lithium on $$left({10ar{1}1} ight)left[{ar{1}012} ight]$$ 10 1. Metals and Materials International, 2018, 24, 720-729.	3.4	6
66	Gaâ€“Doped Ptâ€“Ni Octahedral Nanoparticles as a Highly Active and Durable Electrocatalyst for Oxygen Reduction Reaction. Nano Letters, 2018, 18, 2450-2458.	9.1	125
67	Multiscale Simulation Method for Quantitative Prediction of Surface Wettability at the Atomistic Level. Journal of Physical Chemistry Letters, 2018, 9, 1750-1758.	4.6	23
68	Bifunctional 2D Superlattice Electrocatalysts of Layered Double Hydroxideâ€“Transition Metal Dichalcogenide Active for Overall Water Splitting. ACS Energy Letters, 2018, 3, 952-960.	17.4	140
69	Frontispiece: Î±â€MnO₂ Nanowireâ€Anchored Highly Oxidized Cluster as a Catalyst for Liâ€O₂ Batteries: Superior Electrocatalytic Activity and High Functionality. Angewandte Chemie - International Edition, 2018, 57, .	13.8	1
70	The Achilles' heel of iron-based catalysts during oxygen reduction in an acidic medium. Energy and Environmental Science, 2018, 11, 3176-3182.	30.8	332
71	Frontispiz: Î±â€MnO₂ Nanowireâ€Anchored Highly Oxidized Cluster as a Catalyst for Liâ€O₂ Batteries: Superior Electrocatalytic Activity and High Functionality. Angewandte Chemie, 2018, 130, .	2.0	0
72	Hydration Thermodynamics of Non-Polar Aromatic Hydrocarbons: Comparison of Implicit and Explicit Solvation Models. Molecules, 2018, 23, 2927.	3.8	13

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73	Roles of SnX₂ (X = F, Cl, Br) Additives in Tin-Based Halide Perovskites toward Highly Efficient and Stable Lead-Free Perovskite Solar Cells. Journal of Physical Chemistry Letters, 2018, 9, 6024-6031.	4.6	121
74	Superior role of MXene nanosheet as hybridization matrix over graphene in enhancing interfacial electronic coupling and functionalities of metal oxide. Nano Energy, 2018, 53, 841-848.	16.0	36
75	Solid Electrolyte: Solid Electrolyte Layers by Solution Deposition (Adv. Mater. Interfaces 8/2018). Advanced Materials Interfaces, 2018, 5, 1870035.	3.7	1
76	Î±â€MnO 2 Nanowireâ€Anchored Highly Oxidized Cluster as a Catalyst for Liâ€O 2 Batteries: Superior Electrocatalytic Activity and High Functionality. Angewandte Chemie, 2018, 130, 16216-16221.	2.0	6
77	Î±â€MnO₂ Nanowireâ€Anchored Highly Oxidized Cluster as a Catalyst for Liâ€O₂ Batteries: Superior Electrocatalytic Activity and High Functionality. Angewandte Chemie - International Edition, 2018, 57, 15984-15989.	13.8	76
78	Carbon Monoxide as a Promoter of Atomically Dispersed Platinum Catalyst in Electrochemical Hydrogen Evolution Reaction. Journal of the American Chemical Society, 2018, 140, 16198-16205.	13.7	74
79	Impacts of cation ordering on bandgap dispersion of double perovskites. APL Materials, 2018, 6, .	5.1	14
80	A rational method to kinetically control the rate-determining step to explore efficient electrocatalysts for the oxygen evolution reaction. NPG Asia Materials, 2018, 10, 659-669.	7.9	66
81	Heterolayered 2D nanohybrids of uniformly stacked transition metal dichalcogenideâ€“transition metal oxide monolayers with improved energy-related functionalities. Journal of Materials Chemistry A, 2018, 6, 15237-15244.	10.3	33
82	A hydro/oxo-phobic top hole-selective layer for efficient and stable colloidal quantum dot solar cells. Energy and Environmental Science, 2018, 11, 2078-2084.	30.8	41
83	Molecular Identification of Cr(VI) Removal Mechanism on Vivianite Surface. Environmental Science & Technology, 2018, 52, 10647-10656.	10.0	53
84	Polymorphic Phase Control Mechanism of Organicâ€“Inorganic Hybrid Perovskite Engineered by Dual-Site Alloying. Journal of Physical Chemistry C, 2017, 121, 9508-9515.	3.1	16
85	High-efficiency and high-power rechargeable lithiumâ€“sulfur dioxide batteries exploiting conventional carbonate-based electrolytes. Nature Communications, 2017, 8, 14989.	12.8	40
86	Facile CO₂ Electro-Reduction to Formate via Oxygen Bidentate Intermediate Stabilized by High-Index Planes of Bi Dendrite Catalyst. ACS Catalysis, 2017, 7, 5071-5077.	11.2	263
87	Synergistic interaction of Re complex and amine functionalized multiple ligands in metal-organic frameworks for conversion of carbon dioxide. Scientific Reports, 2017, 7, 612.	3.3	64
88	Nitrate reduction on the surface of bimetallic catalysts supported by nano-crystalline beta-zeolite (NBeta). Green Chemistry, 2017, 19, 853-866.	9.0	38
89	Insight into Electrochemical CO₂ Reduction on Surface-Molecule-Mediated Ag Nanoparticles. ACS Catalysis, 2017, 7, 779-785.	11.2	205
90	Band Gap Engineering of Cs₃Bi₂I₉ Perovskites with Trivalent Atoms Using a Dual Metal Cation. Journal of Physical Chemistry C, 2017, 121, 969-974.	3.1	49

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91	Distorted Carbon Nitride Structure with Substituted Benzene Moieties for Enhanced Visible Light Photocatalytic Activities. ACS Applied Materials & Interfaces, 2017, 9, 40360-40368.	8.0	80
92	Highly selective adsorption of p-xylene over other C₈ aromatic hydrocarbons by Co-CUK-1: a combined experimental and theoretical assessment. Dalton Transactions, 2017, 46, 16096-16101.	3.3	20
93	New Features and Uncovered Benefits of Polycrystalline Magnetite as Reusable Catalyst in Reductive Chemical Conversion. Journal of Physical Chemistry C, 2017, 121, 25195-25205.	3.1	15
94	Transfer and Dynamic Inversion of Coassembled Supramolecular Chirality through 2D-Sheet to Rolled-Up Tubular Structure. Journal of the American Chemical Society, 2017, 139, 17711-17714.	13.7	62
95	Zincâ€“Phosphorus Complex Working as an Atomic Valve for Colloidal Growth of Monodisperse Indium Phosphide Quantum Dots. Chemistry of Materials, 2017, 29, 6346-6355.	6.7	53
96	The Mechanism of Room-Temperature Ionic-Liquid-Based Electrochemical CO2 Reduction: A Review. Molecules, 2017, 22, 536.	3.8	53
97	A Conductive Hybridization Matrix of RuO₂ Twoâ€Dimensional Nanosheets: A Hybridâ€Type Photocatalyst. Angewandte Chemie - International Edition, 2016, 55, 8546-8550.	13.8	48
98	Laser-induced phase separation of silicon carbide. Nature Communications, 2016, 7, 13562.	12.8	75
99	Recent development of atomâ€pairwise van der waals corrections for density functional theory: From molecules to solids. International Journal of Quantum Chemistry, 2016, 116, 598-607.	2.0	19
100	Exfoliated Metal Oxide Nanosheets as Effective and Applicable Substrates for Atomically Dispersed Metal Nanoparticles with Tailorable Functionalities. Advanced Materials Interfaces, 2016, 3, 1600661.	3.7	5
101	2D Covalent Metals: A New Materials Domain of Electrochemical CO₂ Conversion with Broken Scaling Relationship. Journal of Physical Chemistry Letters, 2016, 7, 4124-4129.	4.6	54
102	Failure of Density Functional Dispersion Correction in Metallic Systems and Its Possible Solution Using a Modified Many-Body Dispersion Correction. Journal of Physical Chemistry Letters, 2016, 7, 3278-3283.	4.6	13
103	Highly Efficient, Selective, and Stable CO₂ Electroreduction on a Hexagonal Zn Catalyst. Angewandte Chemie, 2016, 128, 9443-9446.	2.0	61
104	Highly Efficient, Selective, and Stable CO₂ Electroreduction on a Hexagonal Zn Catalyst. Angewandte Chemie - International Edition, 2016, 55, 9297-9300.	13.8	304
105	Probing Distinct Fullerene Formation Processes from Carbon Precursors of Different Sizes and Structures. Analytical Chemistry, 2016, 88, 8232-8238.	6.5	6
106	A Seamless Grid-Based Interface for Mean-Field QM/MM Coupled with Efficient Solvation Free Energy Calculations. Journal of Chemical Theory and Computation, 2016, 12, 5088-5099.	5.3	36
107	Tuning selectivity of electrochemical reactions by atomically dispersed platinum catalyst. Nature Communications, 2016, 7, 10922.	12.8	683
108	Tuned Chemical Bonding Ability of Au at Grain Boundaries for Enhanced Electrochemical CO₂ Reduction. ACS Catalysis, 2016, 6, 4443-4448.	11.2	103

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109	A mechanistic model for hydrogen activation, spillover, and its chemical reaction in a zeolite-encapsulated Pt catalyst. Physical Chemistry Chemical Physics, 2016, 18, 7035-7041.	2.8	38
110	Effect of NaBH 4 on properties of nanoscale zero-valent iron and its catalytic activity for reduction of p -nitrophenol. Applied Catalysis B: Environmental, 2016, 182, 541-549.	20.2	229
111	Hydrogen Spillover in Encapsulated Metal Catalysts: New Opportunities for Designing Advanced Hydroprocessing Catalysts. ChemCatChem, 2015, 7, 1048-1057.	3.7	56
112	Theoretical and Experimental Studies of the Dechlorination Mechanism of Carbon Tetrachloride on a Vivianite Ferrous Phosphate Surface. Journal of Physical Chemistry A, 2015, 119, 5714-5722.	2.5	14
113	Induction and control of supramolecular chirality by light in self-assembled helical nanostructures. Nature Communications, 2015, 6, 6959.	12.8	180
114	Magnetotactic molecular architectures from self-assembly of Î²-peptide foldamers. Nature Communications, 2015, 6, 8747.	12.8	59
115	Achieving Selective and Efficient Electrocatalytic Activity for CO₂ Reduction Using Immobilized Silver Nanoparticles. Journal of the American Chemical Society, 2015, 137, 13844-13850.	13.7	575
116	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. ACS Applied Materials & Interfaces, 2015, 7, 18679-18688.	8.0	53
117	Prediction of the reduction potential of tris(2,2â€²-bipyridinyl)iron(III/II) derivatives. Journal of Computational Chemistry, 2015, 36, 33-41.	3.3	11
118	Rapid Dye Regeneration Mechanism of Dye-Sensitized Solar Cells. Journal of Physical Chemistry Letters, 2014, 5, 4285-4290.	4.6	22
119	Nitrite Reduction Mechanism on a Pd Surface. Environmental Science & Technology, 2014, 48, 12768-12774.	10.0	188
120	Selective Dissociation of Dihydrogen over Dioxygen on a Hindered Platinum Surface for the Direct Synthesis of Hydrogen Peroxide. ChemCatChem, 2014, 6, 2836-2842.	3.7	23
121	Maximizing the catalytic function of hydrogen spillover in platinum-encapsulated aluminosilicates with controlled nanostructures. Nature Communications, 2014, 5, 3370.	12.8	181
122	Embedding Covalency into Metal Catalysts for Efficient Electrochemical Conversion of CO₂. Journal of the American Chemical Society, 2014, 136, 11355-11361.	13.7	192
123	Effect of marine environmental factors on the phase equilibrium of CO2 hydrate. International Journal of Greenhouse Gas Control, 2014, 20, 285-292.	4.6	35
124	Long-Range Electron Transfer over Graphene-Based Catalyst for High-Performing Oxygen Reduction Reactions: Importance of Size, N-doping, and Metallic Impurities. Journal of the American Chemical Society, 2014, 136, 9070-9077.	13.7	288
125	First-Principles Design of Hydrogen Dissociation Catalysts Based on Isoelectronic Metal Solid Solutions. Journal of Physical Chemistry Letters, 2014, 5, 1819-1824.	4.6	26
126	A protocol to evaluate one electron redox potential for iron complexes. Journal of Computational Chemistry, 2013, 34, 2233-2241.	3.3	36

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127	Inner-Sphere Electron-Transfer Single Iodide Mechanism for Dye Regeneration in Dye-Sensitized Solar Cells. Journal of the American Chemical Society, 2013, 135, 2431-2434.	13.7	28
128	DFT Study of Water Adsorption and Decomposition on a Ga-Rich GaP(001)(2Ã—4) Surface. Journal of Physical Chemistry C, 2012, 116, 17604-17612.	3.1	31
129	Turning On MLCT Phosphorescence of Iridium(III)â€“Borane Conjugates upon Fluoride Binding. Organometallics, 2012, 31, 31-34.	2.3	44
130	The Role of Confined Water in Ionic Liquid Electrolytes for Dye-Sensitized Solar Cells. Journal of Physical Chemistry Letters, 2012, 3, 556-559.	4.6	36
131	Anisotropic Shock Sensitivity of Cyclotrimethylene Trinitramine (RDX) from Compress-and-Shear Reactive Dynamics. Journal of Physical Chemistry C, 2012, 116, 10198-10206.	3.1	69
132	Universal Correction of Density Functional Theory to Include London Dispersion (up to Lr, Element) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	4.6	47
133	High-temperature high-pressure phases of lithium from electron force field (eFF) quantum electron dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 15101-15105.	7.1	23
134	Wall-mediated self-diffusion in slit and cylindrical pores. Physical Review E, 2008, 77, 031202.	2.1	9
135	DYNAMICS OF SIMPLE FLUIDS CONFINED IN CYLINDRICAL PORE: EFFECT OF PORE SIZE. Journal of Theoretical and Computational Chemistry, 2005, 04, 305-315.	1.8	7