

Hyungjun Kim

List of Publications by Year in descending order

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135
papers

9,500
citations

38742

50
h-index

40979

93
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all docs

136
docs citations

136
times ranked

12185
citing authors

#	ARTICLE	IF	CITATIONS
1	Tuning selectivity of electrochemical reactions by atomically dispersed platinum catalyst. <i>Nature Communications</i> , 2016, 7, 10922.	12.8	683
2	Achieving Selective and Efficient Electrocatalytic Activity for CO ₂ Reduction Using Immobilized Silver Nanoparticles. <i>Journal of the American Chemical Society</i> , 2015, 137, 13844-13850.	13.7	575
3	Reversible and cooperative photoactivation of single-atom Cu/TiO ₂ photocatalysts. <i>Nature Materials</i> , 2019, 18, 620-626.	27.5	501
4	The Achilles' heel of iron-based catalysts during oxygen reduction in an acidic medium. <i>Energy and Environmental Science</i> , 2018, 11, 3176-3182.	30.8	332
5	Highly Efficient, Selective, and Stable CO ₂ Electroreduction on a Hexagonal Zn Catalyst. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 9297-9300.	13.8	304
6	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> , 2014, 136, 9070-9077.	13.7	288
7	Redirecting dynamic surface restructuring of a layered transition metal oxide catalyst for superior water oxidation. <i>Nature Catalysis</i> , 2021, 4, 212-222.	34.4	266
8	Facile CO ₂ Electro-Reduction to Formate via Oxygen Bidentate Intermediate Stabilized by High-Index Planes of Bi Dendrite Catalyst. <i>ACS Catalysis</i> , 2017, 7, 5071-5077.	11.2	263
9	Effect of NaBH ₄ on properties of nanoscale zero-valent iron and its catalytic activity for reduction of p-nitrophenol. <i>Applied Catalysis B: Environmental</i> , 2016, 182, 541-549.	20.2	229
10	Insight into Electrochemical CO ₂ Reduction on Surface-Molecule-Mediated Ag Nanoparticles. <i>ACS Catalysis</i> , 2017, 7, 779-785.	11.2	205
11	Time-resolved observation of C-C coupling intermediates on Cu electrodes for selective electrochemical CO ₂ reduction. <i>Energy and Environmental Science</i> , 2020, 13, 4301-4311.	30.8	197
12	Embedding Covalency into Metal Catalysts for Efficient Electrochemical Conversion of CO ₂ . <i>Journal of the American Chemical Society</i> , 2014, 136, 11355-11361.	13.7	192
13	Nitrite Reduction Mechanism on a Pd Surface. <i>Environmental Science & Technology</i> , 2014, 48, 12768-12774.	10.0	188
14	Maximizing the catalytic function of hydrogen spillover in platinum-encapsulated aluminosilicates with controlled nanostructures. <i>Nature Communications</i> , 2014, 5, 3370.	12.8	181
15	Induction and control of supramolecular chirality by light in self-assembled helical nanostructures. <i>Nature Communications</i> , 2015, 6, 6959.	12.8	180
16	Bifunctional 2D Superlattice Electrocatalysts of Layered Double Hydroxide-Transition Metal Dichalcogenide Active for Overall Water Splitting. <i>ACS Energy Letters</i> , 2018, 3, 952-960.	17.4	140
17	Ga-Doped Pt-Ni Octahedral Nanoparticles as a Highly Active and Durable Electrocatalyst for Oxygen Reduction Reaction. <i>Nano Letters</i> , 2018, 18, 2450-2458.	9.1	125
18	Roles of SnX ₂ (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> , 2018, 9, 6024-6031.	4.6	121

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19	Polymeric Carbon Nitride with Localized Aluminum Coordination Sites as a Durable and Efficient Photocatalyst for Visible Light Utilization. <i>ACS Catalysis</i> , 2018, 8, 4241-4256.	11.2	118
20	A General Strategy to Atomically Dispersed Precious Metal Catalysts for Unravelling Their Catalytic Trends for Oxygen Reduction Reaction. <i>ACS Nano</i> , 2020, 14, 1990-2001.	14.6	116
21	Intermetallic PtCu Nanoframes as Efficient Oxygen Reduction Electrocatalysts. <i>Nano Letters</i> , 2020, 20, 7413-7421.	9.1	109
22	Identification of Single-Atom Ni Site Active toward Electrochemical CO ₂ Conversion to CO. <i>Journal of the American Chemical Society</i> , 2021, 143, 925-933.	13.7	107
23	Selective electrochemical reduction of nitric oxide to hydroxylamine by atomically dispersed iron catalyst. <i>Nature Communications</i> , 2021, 12, 1856.	12.8	106
24	Tuned Chemical Bonding Ability of Au at Grain Boundaries for Enhanced Electrochemical CO ₂ Reduction. <i>ACS Catalysis</i> , 2016, 6, 4443-4448.	11.2	103
25	Unveiling Electrodeâ€“Electrolyte Design-Based NO Reduction for NH ₃ Synthesis. <i>ACS Energy Letters</i> , 2020, 5, 3647-3656.	17.4	97
26	Activity Origin and Multifunctionality of Pt-Based Intermetallic Nanostructures for Efficient Electrocatalysis. <i>ACS Catalysis</i> , 2019, 9, 11242-11254.	11.2	96
27	High-performance p-channel transistors with transparent Zn doped-CuI. <i>Nature Communications</i> , 2020, 11, 4309.	12.8	94
28	Ultrafast charge transfer coupled with lattice phonons in two-dimensional covalent organic frameworks. <i>Nature Communications</i> , 2019, 10, 1873.	12.8	93
29	On the importance of the electric double layer structure in aqueous electrocatalysis. <i>Nature Communications</i> , 2022, 13, 174.	12.8	92
30	Exfoliated 2D Lepidocrocite Titanium Oxide Nanosheets for High Sulfur Content Cathodes with Highly Stable Liâ€“S Battery Performance. <i>ACS Energy Letters</i> , 2018, 3, 412-419.	17.4	90
31	Electronic interaction between transition metal single-atoms and anatase TiO ₂ boosts CO ₂ photoreduction with H ₂ O. <i>Energy and Environmental Science</i> , 2022, 15, 601-609.	30.8	88
32	Thermal Transformation of Molecular Ni ²⁺ â€“N ₄ Sites for Enhanced CO ₂ Electroreduction Activity. <i>ACS Catalysis</i> , 2020, 10, 10920-10931.	11.2	81
33	Distorted Carbon Nitride Structure with Substituted Benzene Moieties for Enhanced Visible Light Photocatalytic Activities. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 40360-40368.	8.0	80
34	Mixed Valence Perovskite Cs ₂ Au ₂ I ₆ : A Potential Material for Thinâ€“Film Pbâ€“Free Photovoltaic Cells with Ultrahigh Efficiency. <i>Advanced Materials</i> , 2018, 30, e1707001.	21.0	79
35	Insight into the Microenvironments of the Metalâ€“Ionic Liquid Interface during Electrochemical CO ₂ Reduction. <i>ACS Catalysis</i> , 2018, 8, 2420-2427.	11.2	77
36	â€“MnO ₂ Nanowireâ€“Anchored Highly Oxidized Cluster as a Catalyst for Liâ€“O ₂ Batteries: Superior Electrocatalytic Activity and High Functionality. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 15984-15989.	13.8	76

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37	Laser-induced phase separation of silicon carbide. <i>Nature Communications</i> , 2016, 7, 13562.	12.8	75
38	Carbon Monoxide as a Promoter of Atomically Dispersed Platinum Catalyst in Electrochemical Hydrogen Evolution Reaction. <i>Journal of the American Chemical Society</i> , 2018, 140, 16198-16205.	13.7	74
39	Anisotropic Shock Sensitivity of Cyclotrimethylene Trinitramine (RDX) from Compress-and-Shear Reactive Dynamics. <i>Journal of Physical Chemistry C</i> , 2012, 116, 10198-10206.	3.1	69
40	A rational method to kinetically control the rate-determining step to explore efficient electrocatalysts for the oxygen evolution reaction. <i>NPG Asia Materials</i> , 2018, 10, 659-669.	7.9	66
41	Synergistic interaction of Re complex and amine functionalized multiple ligands in metal-organic frameworks for conversion of carbon dioxide. <i>Scientific Reports</i> , 2017, 7, 612.	3.3	64
42	Transfer and Dynamic Inversion of Coassembled Supramolecular Chirality through 2D-Sheet to Rolled-Up Tubular Structure. <i>Journal of the American Chemical Society</i> , 2017, 139, 17711-17714.	13.7	62
43	Metal-Oxide Interfaces for Selective Electrochemical C-C Coupling Reactions. <i>ACS Energy Letters</i> , 2019, 4, 2241-2248.	17.4	62
44	Highly Efficient, Selective, and Stable CO ₂ Electroreduction on a Hexagonal Zn Catalyst. <i>Angewandte Chemie</i> , 2016, 128, 9443-9446.	2.0	61
45	Magnetotactic molecular architectures from self-assembly of β -peptide foldamers. <i>Nature Communications</i> , 2015, 6, 8747.	12.8	59
46	Hydrogen Spillover in Encapsulated Metal Catalysts: New Opportunities for Designing Advanced Hydroprocessing Catalysts. <i>ChemCatChem</i> , 2015, 7, 1048-1057.	3.7	56
47	Monolayered g-C ₃ N ₄ nanosheet as an emerging cationic building block for bifunctional 2D superlattice hybrid catalysts with controlled defect structures. <i>Applied Catalysis B: Environmental</i> , 2020, 277, 119191.	20.2	56
48	2D Covalent Metals: A New Materials Domain of Electrochemical CO ₂ Conversion with Broken Scaling Relationship. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4124-4129.	4.6	54
49	Interface rich CuO/Al ₂ O ₃ /CuO surface for selective ethylene production from electrochemical CO ₂ conversion. <i>Energy and Environmental Science</i> , 2022, 15, 2397-2409.	30.8	54
50	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 & Interfaces</i> , 2015, 7, 18679-18688.	8.0	53
51	Zinc-Phosphorus Complex Working as an Atomic Valve for Colloidal Growth of Monodisperse Indium Phosphide Quantum Dots. <i>Chemistry of Materials</i> , 2017, 29, 6346-6355.	6.7	53
52	The Mechanism of Room-Temperature Ionic-Liquid-Based Electrochemical CO ₂ Reduction: A Review. <i>Molecules</i> , 2017, 22, 536.	3.8	53
53	Molecular Identification of Cr(VI) Removal Mechanism on Vivianite Surface. <i>Environmental Science & Technology</i> , 2018, 52, 10647-10656.	10.0	53
54	Dynamic metal-polymer interaction for the design of chemoselective and long-lived hydrogenation catalysts. <i>Science Advances</i> , 2020, 6, eabb7369.	10.3	53

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55	Band Gap Engineering of Cs ₃ Bi ₂ I ₉ Perovskites with Trivalent Atoms Using a Dual Metal Cation. Journal of Physical Chemistry C, 2017, 121, 969-974.	3.1	49
56	Activity-Stability Relationship in Au@Pt Nanoparticles for Electrocatalysis. ACS Energy Letters, 2020, 5, 2827-2834.	17.4	49
57	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
58	A Conductive Hybridization Matrix of RuO ₂ Two-Dimensional Nanosheets: A Hybrid-Type Photocatalyst. Angewandte Chemie - International Edition, 2016, 55, 8546-8550.	13.8	48
59	Universal Correction of Density Functional Theory to Include London Dispersion (up to Lr, Element) Tj ETQq1 1 0.784314 rgBJ ₄ /Overl	4.6	47
60	Porous Metal-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
61	Turning On MLCT Phosphorescence of Iridium(III)-Borane Conjugates upon Fluoride Binding. Organometallics, 2012, 31, 31-34.	2.3	44
62	Solid Electrolyte Layers by Solution Deposition. Advanced Materials Interfaces, 2018, 5, 1701328.	3.7	42
63	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
64	Fe _x Ni _{2-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
65	Electric Field Mediated Selectivity Switching of Electrochemical CO ₂ Reduction from Formate to CO on Carbon Supported Sn. ACS Energy Letters, 2020, 5, 2987-2994.	17.4	41
66	High-efficiency and high-power rechargeable lithium-sulfur dioxide batteries exploiting conventional carbonate-based electrolytes. Nature Communications, 2017, 8, 14989.	12.8	40
67	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
68	Nitrate reduction on the surface of bimetallic catalysts supported by nano-crystalline beta-zeolite (NBeta). Green Chemistry, 2017, 19, 853-866.	9.0	38
69	Structure, Dynamics, and Wettability of Water at Metal Interfaces. Scientific Reports, 2019, 9, 14805.	3.3	38
70	Benchmarking several van der Waals dispersion approaches for the description of intermolecular interactions. Journal of Chemical Physics, 2018, 148, 064112.	3.0	37
71	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
72	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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73	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> , 2016, 12, 5088-5099.	5.3	36
74	Superior role of MXene nanosheet as hybridization matrix over graphene in enhancing interfacial electronic coupling and functionalities of metal oxide. <i>Nano Energy</i> , 2018, 53, 841-848.	16.0	36
75	<i>Operando</i> Stability of Platinum Electrocatalysts in Ammonia Oxidation Reactions. <i>ACS Catalysis</i> , 2020, 10, 11674-11684.	11.2	36
76	Effect of marine environmental factors on the phase equilibrium of CO ₂ hydrate. <i>International Journal of Greenhouse Gas Control</i> , 2014, 20, 285-292.	4.6	35
77	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> , 2018, 6, 15237-15244.	10.3	33
78	DFT Study of Water Adsorption and Decomposition on a Ga-Rich GaP(001)(2 \times 4) Surface. <i>Journal of Physical Chemistry C</i> , 2012, 116, 17604-17612.	3.1	31
79	μ MBD: A Materials-Ready Dispersion Correction That Uniformly Treats Metallic, Ionic, and van der Waals Bonding. <i>Journal of the American Chemical Society</i> , 2020, 142, 2346-2354.	13.7	29
80	Inner-Sphere Electron-Transfer Single Iodide Mechanism for Dye Regeneration in Dye-Sensitized Solar Cells. <i>Journal of the American Chemical Society</i> , 2013, 135, 2431-2434.	13.7	28
81	Selectivity Modulated by Surface Ligands on Cu ₂ O/TiO ₂ Catalysts for Gas-Phase Photocatalytic Reduction of Carbon Dioxide. <i>Journal of Physical Chemistry C</i> , 2019, 123, 29184-29191.	3.1	27
82	Reversible Ligand Exchange in Atomically Dispersed Catalysts for Modulating the Activity and Selectivity of the Oxygen Reduction Reaction. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 20528-20534.	13.8	27
83	First-Principles Design of Hydrogen Dissociation Catalysts Based on Isoelectronic Metal Solid Solutions. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1819-1824.	4.6	26
84	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 ₂ Batteries. <i>Small</i> , 2020, 16, 1903265.	10.0	26
85	Thermodynamics of Multicomponent Perovskites: A Guide to Highly Efficient and Stable Solar Cell Materials. <i>Chemistry of Materials</i> , 2020, 32, 4265-4272.	6.7	26
86	Electrochemical Evidence for Two Subfamilies of FeN _x C _y Moieties with Concentration-Dependent Cyanide Poisoning. <i>ChemElectroChem</i> , 2018, 5, 1880-1885.	3.4	24
87	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> , 2021, 143, 3113-3123.	13.7	24
88	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> , 2011, 108, 15101-15105.	7.1	23
89	Selective Dissociation of Dihydrogen over Dioxygen on a Hindered Platinum Surface for the Direct Synthesis of Hydrogen Peroxide. <i>ChemCatChem</i> , 2014, 6, 2836-2842.	3.7	23
90	Multiscale Simulation Method for Quantitative Prediction of Surface Wettability at the Atomistic Level. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1750-1758.	4.6	23

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91	Rapid Dye Regeneration Mechanism of Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 4285-4290.	4.6	22
92	Spectroscopic capture of a low-spin Mn(IV)-oxo species in Ni ²⁺ /Mn ₃ O ₄ nanoparticles during water oxidation catalysis. <i>Nature Communications</i> , 2020, 11, 5230.	12.8	21
93	Highly selective adsorption of <i>p</i> -xylene over other C ₈ aromatic hydrocarbons by Co-CUK-1: a combined experimental and theoretical assessment. <i>Dalton Transactions</i> , 2017, 46, 16096-16101.	3.3	20
94	Simultaneous Enhanced Efficiency and Stability of Perovskite Solar Cells Using Adhesive Fluorinated Polymer Interfacial Material. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 35595-35605.	8.0	20
95	Recent development of atom-pairwise van der waals corrections for density functional theory: From molecules to solids. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 598-607.	2.0	19
96	Understanding the relative efficacies and versatile roles of 2D conductive nanosheets in hybrid-type photocatalyst. <i>Applied Catalysis B: Environmental</i> , 2019, 257, 117875.	20.2	19
97	Tailoring a Dynamic Metal-Polymer Interaction to Improve Catalyst Selectivity and Longevity in Hydrogenation. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 12482-12489.	13.8	19
98	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> , 2022, 9, e2103042.	11.2	19
99	Cluster Expansion Method for Simulating Realistic Size of Nanoparticle Catalysts with an Application in CO ₂ Electroreduction. <i>Journal of Physical Chemistry C</i> , 2018, 122, 9245-9254.	3.1	17
100	Ligand-Controlled Direct Hydroformylation of Trisubstituted Olefins. <i>Organic Letters</i> , 2019, 21, 5789-5792.	4.6	17
101	Triphasic Metal Oxide Photocatalyst for Reaction Site-Specific Production of Hydrogen Peroxide from Oxygen Reduction and Water Oxidation. <i>Advanced Energy Materials</i> , 2022, 12, .	19.5	17
102	Polymorphic Phase Control Mechanism of Organic-Inorganic Hybrid Perovskite Engineered by Dual-Site Alloying. <i>Journal of Physical Chemistry C</i> , 2017, 121, 9508-9515.	3.1	16
103	Experimental and Density Functional Theory Corroborated Optimization of Durable Metal Embedded Carbon Nanofiber for Oxygen Electrocatalysis. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3109-3114.	4.6	16
104	Enthalpy-Entropy Interplay in π -Stacking Interaction of Benzene Dimer in Water. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1538-1545.	5.3	16
105	New Features and Uncovered Benefits of Polycrystalline Magnetite as Reusable Catalyst in Reductive Chemical Conversion. <i>Journal of Physical Chemistry C</i> , 2017, 121, 25195-25205.	3.1	15
106	Effect of groundwater ions (Ca ²⁺ , Na ⁺ , and HCO ₃ ⁻) on removal of hexavalent chromium by Fe(II)-phosphate mineral. <i>Journal of Hazardous Materials</i> , 2020, 398, 122948.	12.4	15
107	Theoretical and Experimental Studies of the Dechlorination Mechanism of Carbon Tetrachloride on a Vivianite Ferrous Phosphate Surface. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5714-5722.	2.5	14
108	Impacts of cation ordering on bandgap dispersion of double perovskites. <i>APL Materials</i> , 2018, 6, .	5.1	14

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109	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> , 2016, 7, 3278-3283.	4.6	13
110	Hydration Thermodynamics of Non-Polar Aromatic Hydrocarbons: Comparison of Implicit and Explicit Solvation Models. <i>Molecules</i> , 2018, 23, 2927.	3.8	13
111	Electronic Structure and Band Alignments of Various Phases of Titania Using the Self-Consistent Hybrid Density Functional and DFT+U Methods. <i>Frontiers in Chemistry</i> , 2019, 7, 47.	3.6	12
112	Light Emission Enhancement by Tuning the Structural Phase of APbBr ₃ (A =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 627 Td (2135-2142.	4.6	12
113	Prediction of the reduction potential of tris(2,2'-bipyridinyl)iron(III/II) derivatives. <i>Journal of Computational Chemistry</i> , 2015, 36, 33-41.	3.3	11
114	Microbially Guided Discovery and Biosynthesis of Biologically Active Natural Products. <i>ACS Synthetic Biology</i> , 2021, 10, 1505-1519.	3.8	11
115	Self-Assembly of a Peptide Foldamer: The Role of the Surfactant in Three-Dimensional Shape Selection. <i>ChemPlusChem</i> , 2019, 84, 481-487.	2.8	10
116	Wall-mediated self-diffusion in slit and cylindrical pores. <i>Physical Review E</i> , 2008, 77, 031202.	2.1	9
117	Physicochemical Understanding of the Impact of Pore Environment and Species of Adsorbates on Adsorption Behaviour. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 20504-20510.	13.8	8
118	DYNAMICS OF SIMPLE FLUIDS CONFINED IN CYLINDRICAL PORE: EFFECT OF PORE SIZE. <i>Journal of Theoretical and Computational Chemistry</i> , 2005, 04, 305-315.	1.8	7
119	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> , 2022, 43, 476-483.	1.9	7
120	Probing Distinct Fullerene Formation Processes from Carbon Precursors of Different Sizes and Structures. <i>Analytical Chemistry</i> , 2016, 88, 8232-8238.	6.5	6
121	First-Principles Studies on Twinnability of Magnesium Alloys: Effects of Yttrium and Lithium on $\left(\{10\bar{1}1\} \right) \left[\{11\bar{2}0\} \right]$. <i>Metals and Materials International</i> , 2018, 24, 720-729.	3.4	6
122	MnO ₂ Nanowire-Anchored Highly Oxidized Cluster as a Catalyst for Li-O ₂ Batteries: Superior Electrocatalytic Activity and High Functionality. <i>Angewandte Chemie</i> , 2018, 130, 16216-16221.	2.0	6
123	Water Slippage on Graphitic and Metallic Surfaces: Impact of the Surface Packing Structure and Electron Density Tail. <i>Journal of Physical Chemistry C</i> , 2020, 124, 11392-11400.	3.1	6
124	Exfoliated Metal Oxide Nanosheets as Effective and Applicable Substrates for Atomically Dispersed Metal Nanoparticles with Tailorable Functionalities. <i>Advanced Materials Interfaces</i> , 2016, 3, 1600661.	3.7	5
125	<i>In Situ</i> Mapping and Local Negative Uptake Behavior of Adsorbates in Individual Pores of Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2021, 143, 20747-20757.	13.7	5
126	Enhanced Light Emission through Symmetry Engineering of Halide Perovskites. <i>Journal of the American Chemical Society</i> , 2022, 144, 297-305.	13.7	5

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127	Reversible Ligand Exchange in Atomically Dispersed Catalysts for Modulating the Activity and Selectivity of the Oxygen Reduction Reaction. <i>Angewandte Chemie</i> , 2021, 133, 20691-20697.	2.0	3
128	Frontispiece: MnO_2 Nanowire-Anchored Highly Oxidized Cluster as a Catalyst for LiO_2 Batteries: Superior Electrocatalytic Activity and High Functionality. <i>Angewandte Chemie - International Edition</i> , 2018, 57, .	13.8	1
129	Solid Electrolyte: Solid Electrolyte Layers by Solution Deposition (<i>Adv. Mater. Interfaces</i> 8/2018). <i>Advanced Materials Interfaces</i> , 2018, 5, 1870035.	3.7	1
130	Electrocatalysts: Synergistic Control of Structural Disorder and Surface Bonding Nature to Optimize the Functionality of Manganese Oxide as an Electrocatalyst and a Cathode for LiO_2 Batteries (<i>Small</i> 12/2020). <i>Small</i> , 2020, 16, 2070062.	10.0	1
131	Femtosecond Quantum Dynamics of Excited-State Evolution of Halide Perovskites: Quantum Chaos of Molecular Cations. <i>Journal of Physical Chemistry C</i> , 2021, 125, 10676-10684.	3.1	1
132	Assessment and prediction of band edge locations of nitrides using a self-consistent hybrid functional. <i>Journal of Chemical Physics</i> , 2021, 155, 024120.	3.0	1
133	Frontispiz: MnO_2 Nanowire-Anchored Highly Oxidized Cluster as a Catalyst for LiO_2 Batteries: Superior Electrocatalytic Activity and High Functionality. <i>Angewandte Chemie</i> , 2018, 130, .	2.0	0
134	Probing Surface Chemistry at an Atomic Level: Decomposition of 1-Propanethiol on GaP(001) (2 Å– 4) Investigated by STM, XPS, and DFT. <i>Journal of Physical Chemistry C</i> , 2019, 123, 2964-2972.	3.1	0
135	Tailoring a Dynamic Metal-Polymer Interaction to Improve Catalyst Selectivity and Longevity in Hydrogenation. <i>Angewandte Chemie</i> , 2021, 133, 12590-12597.	2.0	0