Byungchan Han

List of Publications by Year
in descending order

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103 papers	3,719 citations	126708 33 h-index	143772 57 g-index
107 all docs	107 docs citations	107 times ranked	5644 citing authors

#	Article	IF	Citations
1	Accelerated N2 reduction kinetics in hybrid interfaces of NbTiO4 and nitrogen-doped carbon nanorod via synergistic electronic coupling effect. Applied Catalysis B: Environmental, 2022, 304, 120938.	10.8	23
2	Slow excitonic carrier cooling in Sr-doped PbS nanocrystals for hot carrier devices: an integrated experimental and first-principles approach. Journal of Materials Chemistry C, 2022, 10, 6634-6645.	2.7	3
3	Theoretical Investigation of the Active Sites in N-Doped Graphene Bilayer for the Oxygen Reduction Reaction in Alkaline Media in PEMFCs. Journal of Physical Chemistry C, 2022, 126, 5863-5872.	1.5	8
4	Two-Dimensional Palladium Phosphoronitride for Oxygen Reduction. ACS Applied Materials & Interfaces, 2022, 14, 12156-12167.	4.0	10
5	3â€Dimensional Scanning of Entire Unit Cells in Single Nanoparticles.. ChemNanoMat, 2022, 8, .	1.5	0
6	Metastable hexagonal close-packed palladium hydride in liquid cell TEM. Nature, 2022, 603, 631-636.	13.7	31
7	DFT calculations and machine learning approach to predict catalytic properties of nanoscale electrocatalysts in solution for clean fuel generation. , 2022, 2, 100019.		0
8	Outstanding stability of Gd-doped UO2 against surface oxidation: First-principles study. Applied Surface Science, 2022, 589, 152955.	3.1	1
9	Tuning the electronic structure and inverse degree of inverse spinel ferrites by integrating samarium orthoferrite for efficient water oxidation. Applied Catalysis B: Environmental, 2022, 315, 121504.	10.8	15
10	N- and B-doped fullerene as peroxidase- and catalase-like metal-free nanozymes with pH-switchable catalytic activity: A first-principles approach. Applied Surface Science, 2022, 598, 153715.	3.1	17
11	Efficient removal of 2-chloroethyl ethyl sulfide in solution under solar light by magnesium oxide-decorated polymeric carbon nitride photocatalysts and mechanism investigation. Environmental Advances, 2022, 9, 100255.	2.2	4
12	Selective removal of radioactive iodine from water using reusable Fe@Pt adsorbents. Water Research, 2022, 222, 118864.	5.3	17
13	Tuning the Site-to-Site Interaction in Ruâ€“M (MÂ=ÂCo, Fe, Ni) Diatomic Electrocatalysts to Climb up the Volcano Plot of Oxygen Electroreduction. ACS Nano, 2022, 16, 10657-10666.	7.3	31
14	High quantum efficiency and stability of biohybrid quantum dots nanojunctions in bacteriophage-constructed perovskite. Materials Today Nano, 2021, 13, 100099.	2.3	9
15	Catalytic activity of Ni3Mo surfaces for hydrogen evolution reaction: A density functional theory approach. Applied Surface Science, 2021, 537, 147894.	3.1	25
16	Design of a unique anion framework in halospinels for outstanding performance of all solid-state Li-ion batteries: first-principles approach. Journal of Materials Chemistry A, 2021, 9, 15605-15612.	5.2	12
17	Two-dimensional palladium diselenide for the oxygen reduction reaction. Materials Chemistry Frontiers, 2021, 5, 4970-4980.	3.2	5
18	Pore Tuning of Metalâ€Organic Framework Membrane Anchored on Grapheneâ€Oxide Nanoribbon. Advanced Functional Materials, 2021, 31, 2011146.	7.8	29

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19	Ni nanoparticles on active (001) facet-exposed rutile TiO2 nanopyramid arrays for efficient hydrogen evolution. Applied Catalysis B: Environmental, 2021, 282, 119548.	10.8	40
20	Optical bioelectronic nose of outstanding sensitivity and selectivity toward volatile organic compounds implemented with genetically engineered bacteriophage: Integrated study of multi-scale computational prediction and experimental validation. Biosensors and Bioelectronics, 2021, 177, 112979.	5.3	20
21	Unraveling the selective etching mechanism of silicon nitride over silicon dioxide by phosphoric acid: First-principles study. Applied Surface Science, 2021, 551, 149376.	3.1	10
22	First-Principles-Based Machine-Learning Molecular Dynamics for Crystalline Polymers with van der Waals Interactions. Journal of Physical Chemistry Letters, 2021, 12, 6000-6006.	2.1	14
23	Laserâ€Ablated Red Phosphorus on Carbon Nanotube Film for Accelerating Polysulfide Conversion toward Highâ€Performance and Flexible Lithiumâ€“Sulfur Batteries. Small Methods, 2021, 5, e2100215.	4.6	19
24	Fluorine-Decorated Graphene Nanoribbons for an Anticorrosive Polymer Electrolyte Membrane Fuel Cell. ACS Applied Materials & Interfaces, 2021, 13, 26936-26947.	4.0	18
25	Interfacing or Doping? Role of Ce in Highly Promoted Water Oxidation of NiFeâ€Layered Double Hydroxide. Advanced Energy Materials, 2021, 11, 2101281.	10.2	120
26	First-principle-data-integrated machine-learning approach for high-throughput searching of ternary electrocatalyst toward oxygen reduction reaction. Chem Catalysis, 2021, 1, 855-869.	2.9	28
27	Genetic Manipulation of M13 Bacteriophage for Enhancing the Efficiency of Virusâ€Inoculated Perovskite Solar Cells with a Certified Efficiency of 22.3%. Advanced Energy Materials, 2021, 11, 2101221.	10.2	20
28	n-Type thermoelectric properties of a hexagonal SiGe polymorph superior to a cubic SiGe. Journal of Alloys and Compounds, 2021, 874, 160007.	2.8	5
29	Dramatic catalytic activation of kinetically inert disilane hydrolysis in metallic iron particulate via barrierless chemical dissociation: First-principles study. Applied Surface Science, 2021, 560, 149988.	3.1	3
30	Genetic Manipulation of M13 Bacteriophage for Enhancing the Efficiency of Virusâ€Inoculated Perovskite Solar Cells with a Certified Efficiency of 22.3% (Adv. Energy Mater. 38/2021). Advanced Energy Materials, 2021, 11, 2170150.	10.2	1
31	Desulfurization of hexyl sulfide and hexanethiol using supercritical water. Journal of Supercritical Fluids, 2020, 158, 104734.	1.6	6
32	First-principles computational study of Ni/Î±-Al2O3 hybrid interface reactions under extreme thermodynamic conditions. Applied Surface Science, 2020, 509, 144861.	3.1	3
33	Metal-Induced Self-Assembly Template for Controlled Growth of ZIF-8 Nanorods. Chemistry of Materials, 2020, 32, 7941-7950.	3.2	31
34	Defect structure evolution of polyacrylonitrile and single wall carbon nanotube nanocomposites: a molecular dynamics simulation approach. Scientific Reports, 2020, 10, 11816.	1.6	7
35	Dominant effect of anharmonicity on the equation of state and thermal conductivity of MgO under extreme conditions. Physical Review B, 2020, 102, .	1.1	7
36	Copper phosphosulfides as a highly active and stable photocatalyst for hydrogen evolution reaction. Applied Catalysis B: Environmental, 2020, 273, 118927.	10.8	28

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37	Critical differences in 3D atomic structure of individual ligand-protected nanocrystals in solution. Science, 2020, 368, 60-67.	6.0	103
38	Pairing of Transition Metal Dichalcogenides and Doped Graphene for Catalytically Dual Active Interfaces for the Hydrogen Evolution Reaction. ACS Sustainable Chemistry and Engineering, 2020, , .	3.2	0
39	Thermochemical study for remediation of highly concentrated acid spill: Computational modeling and experimental validation. Chemosphere, 2020, 247, 126098.	4.2	2
40	Sizeâ€Extensive Molecular Machine Learning with Global Representations. ChemSystemsChem, 2020, 2, e1900052.	1.1	20
41	First-Principles Design of Highly Functional Sulfide Electrolyte of Li_{10â^'x}SnP₂S_{12â^'x}Cl_x for All Solid-State Li-Ion Battery Applications. ACS Sustainable Chemistry and Engineering, 2020, 8, 3321-3327.	3.2	26
42	First-principles mechanism study on distinct optoelectronic properties of Cl-doped 2D hybrid tin iodide perovskite. Journal of Materials Chemistry C, 2020, 8, 9540-9548.	2.7	21
43	Ultrastable molybdenum disulfide-based electrocatalyst for hydrogen evolution in acidic media. Journal of Power Sources, 2020, 456, 227998.	4.0	23
44	Unique design of superior metal-organic framework for removal of toxic chemicals in humid environment via direct functionalization of the metal nodes. Journal of Hazardous Materials, 2020, 398, 122857.	6.5	28
45	Design of highly efficient adsorbents for removal of gaseous methyl iodide using tertiary amine-impregnated activated carbon: Integrated experimental and first-principles approach. Chemical Engineering Journal, 2019, 373, 1003-1011.	6.6	27
46	Integrated study of experiment and firstâ€principles computation for the characterization of a corium type ZrO ₈ complex in a Zrâ€doped fluorite UO ₂. International Journal of Energy Research, 2019, 43, 3322-3329.	2.2	8
47	Design of active bifunctional electrocatalysts using single atom doped transition metal dichalcogenides. Applied Surface Science, 2019, 471, 545-552.	3.1	67
48	Elucidation of hydrolysis reaction mechanism of tungsten hexafluoride (WF6) using first-principles calculations. Journal of Industrial and Engineering Chemistry, 2019, 70, 99-102.	2.9	4
49	Unexpectedly high energy density of a Li-Ion battery by oxygen redox in LiNiO2 cathode: First-principles study. Electrochimica Acta, 2019, 294, 166-172.	2.6	27
50	First-principles computational design of unknown flat arsenene epitaxially grown on copper substrate. Applied Surface Science, 2019, 467-468, 561-566.	3.1	15
51	First-principles prediction of universal relation between exchange current density and adsorption energy of rare-earth elements in a molten salt. Journal of Industrial and Engineering Chemistry, 2019, 70, 94-98.	2.9	2
52	First principles computational studies of spontaneous reduction reaction of Eu(III) in eutectic LiCl-KCl molten salt. International Journal of Energy Research, 2018, 42, 2757-2765.	2.2	14
53	High Activity Hydrogen Evolution Catalysis by Uniquely Designed Amorphous/Metal Interface of Coreâ€“shell Phosphosulfide/Nâ€Doped CNTs. Advanced Energy Materials, 2018, 8, 1702806.	10.2	39
54	First-Principles Computational Screening of Highly Active Pyrites Catalysts for Hydrogen Evolution Reaction through a Universal Relation with a Thermodynamic Variable. Journal of Physical Chemistry C, 2018, 122, 2107-2112.	1.5	18

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55	Universal Scaling Relationship To Screen an Efficient Metallic Adsorbent for Adsorptive Removal of Iodine Gas under Humid Conditions: First-Principles Study. Journal of Physical Chemistry C, 2018, 122, 11799-11806.	1.5	7
56	First-principles study on thermodynamic stability of the hybrid interfacial structure of LiMn₂O₄ cathode and carbonate electrolyte in Li-ion batteries. Physical Chemistry Chemical Physics, 2018, 20, 11592-11597.	1.3	19
57	First principles computational study on hydrolysis of hazardous chemicals phosphorus trichloride and oxychloride (PCl3 and POCl3) catalyzed by molecular water clusters. Journal of Hazardous Materials, 2018, 341, 457-463.	6.5	13
58	First-principles computational approach for innovative design of highly functional electrocatalysts in fuel cells. Current Opinion in Electrochemistry, 2018, 12, 225-232.	2.5	4
59	Electrocatalytic activity of electrochemically dealloyed PdCu₃ intermetallic compound towards oxygen reduction reaction in acidic media. Journal of Materials Chemistry A, 2018, 6, 14828-14837.	5.2	49
60	First-principles database driven computational neural network approach to the discovery of active ternary nanocatalysts for oxygen reduction reaction. Physical Chemistry Chemical Physics, 2018, 20, 24539-24544.	1.3	37
61	Tuning the catalytic activity of heterogeneous two-dimensional transition metal dichalcogenides for hydrogen evolution. Journal of Materials Chemistry A, 2018, 6, 20005-20014.	5.2	63
62	Bifunctionally active and durable hierarchically porous transition metal-based hybrid electrocatalyst for rechargeable metal-air batteries. Applied Catalysis B: Environmental, 2018, 239, 677-687.	10.8	64
63	The effect of alloying of transition metals (MÂ= Fe, Co, Ni) with palladium catalysts on the electrocatalytic activity for the oxygen reduction reaction in alkaline media. Electrochimica Acta, 2018, 283, 1045-1052.	2.6	30
64	Synthesis of Durable Small-sized Bilayer Au@Pt Nanoparticles for High Performance PEMFC Catalysts. Electrochimica Acta, 2017, 228, 389-397.	2.6	18
65	Specific approaches to dramatic reduction in stack activation time and perfect long-term storage for high-performance air-breathing polymer electrolyte membrane fuel cell. International Journal of Hydrogen Energy, 2017, 42, 16288-16293.	3.8	6
66	Self-assembled nitrogen-doped fullerenes and their catalysis for fuel cell and rechargeable metalâ€“air battery applications. Nanoscale, 2017, 9, 7373-7379.	2.8	56
67	Enhanced Electrocatalytic Activity of Carbon-Supported Ordered Intermetallic Palladiumâ€“Lead (Pd₃Pb) Nanoparticles toward Electrooxidation of Formic Acid. Chemistry of Materials, 2017, 29, 2906-2913.	3.2	73
68	Effective Trapping of Lithium Polysulfides Using a Functionalized Carbon Nanotube-Coated Separator for Lithiumâ€“Sulfur Cells with Enhanced Cycling Stability. ACS Applied Materials & Interfaces, 2017, 9, 38445-38454.	4.0	82
69	Carrier scattering in quasi-free standing graphene on hexagonal boron nitride. Nanoscale, 2017, 9, 15934-15944.	2.8	7
70	First-Principles Design of Graphene-Based Active Catalysts for Oxygen Reduction and Evolution Reactions in the Aprotic Liâ€“O₂ Battery. Journal of Physical Chemistry Letters, 2016, 7, 2803-2808.	2.1	52
71	First principles study of the thermodynamic and kinetic properties of U in an electrorefining system using molybdenum cathode and LiCl-KCl eutectic molten salt. Electrochimica Acta, 2016, 195, 216-222.	2.6	26
72	Towards a comprehensive understanding of FeCo coated with N-doped carbon as a stable bi-functional catalyst in acidic media. NPG Asia Materials, 2016, 8, e312-e312.	3.8	82

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73	Fast stack activation procedure and effective long-term storage for high-performance polymer electrolyte membrane fuel cell. Journal of Power Sources, 2016, 328, 75-80.	4.0	11
74	Experimental Growth of New 6-fold Symmetry Patterned Microcrystals of AlN: Equilibrium Structures and Growth Mechanism. Crystal Growth and Design, 2016, 16, 5305-5311.	1.4	19
75	Oxygen-Deficient Zirconia (ZrO2â^'x): A New Material for Solar Light Absorption. Scientific Reports, 2016, 6, 27218.	1.6	250
76	First principles computational study on the adsorption mechanism of organic methyl iodide gas on triethylenediamine impregnated activated carbon. Physical Chemistry Chemical Physics, 2016, 18, 32050-32056.	1.3	32
77	Increasing strength and conductivity of Cu alloy through abnormal plastic deformation of an intermetallic compound. Scientific Reports, 2016, 6, 30907.	1.6	40
78	First-principles based computational study on nucleation and growth mechanisms of U on Mo(110) surface solvated in an eutectic LiCl-KCl molten salt. International Journal of Energy Research, 2016, 40, 1381-1388.	2.2	13
79	First-Principles Characterization of the Unknown Crystal Structure and Ionic Conductivity of Li₇P₂S₈I as a Solid Electrolyte for High-Voltage Li Ion Batteries. Journal of Physical Chemistry Letters, 2016, 7, 2671-2675.	2.1	37
80	A New Family of Perovskite Catalysts for Oxygen-Evolution Reaction in Alkaline Media: BaNiO₃and BaNi_{0.83}O_{2.5}. Journal of the American Chemical Society, 2016, 138, 3541-3547.	6.6	204
81	Reliable and cost effective design of intermetallic Ni2Si nanowires and direct characterization of its mechanical properties. Scientific Reports, 2015, 5, 15050.	1.6	19
82	Design of exceptionally strong and conductive Cu alloys beyond the conventional speculation via the interfacial energy-controlled dispersion of Î³-Al2O3 nanoparticles. Scientific Reports, 2015, 5, 17364.	1.6	31
83	First-Principles Study on the Thermal Stability of LiNiO₂ Materials Coated by Amorphous Al₂O₃ with Atomic Layer Thickness. ACS Applied Materials & Interfaces, 2015, 7, 11599-11603.	4.0	47
84	Improved Corrosion Resistance and Mechanical Properties of CrN Hard Coatings with an Atomic Layer Deposited Al₂O₃ Interlayer. ACS Applied Materials & Interfaces, 2015, 7, 26716-26725.	4.0	69
85	Integrated study of first principles calculations and experimental measurements for Li-ionic conductivity in Al-doped solid-state LiGe2(PO4)3 electrolyte. Journal of Power Sources, 2015, 293, 11-16.	4.0	73
86	First-principles computational study of highly stable and active ternary PtCuNi nanocatalyst for oxygen reduction reaction. Nano Research, 2015, 8, 3394-3403.	5.8	46
87	Design of an active and durable catalyst for oxygen reduction reactions using encapsulated Cu with N-doped carbon shells (Cu@N-C) activated by CO₂ treatment. Journal of Materials Chemistry A, 2015, 3, 22031-22034.	5.2	77
88	First Principles Study of Morphology, Doping Level, and Water Solvation Effects on the Catalytic Mechanism of Nitrogenâ€Doped Graphene in the Oxygen Reduction Reaction. ChemCatChem, 2014, 6, 2662-2670.	1.8	40
89	Multi-scale computational study of the molten salt based recycling of spent nuclear fuels. International Journal of Energy Research, 2014, 38, 1987-1993.	2.2	10
90	Toward New Fuel Cell Support Materials: A Theoretical and Experimental Study of Nitrogenâ€Doped Graphene. ChemSusChem, 2014, 7, 2609-2620.	3.6	45

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91	Theoretical insight into highly durable iron phthalocyanine derived non-precious catalysts for oxygen reduction reactions. Journal of Materials Chemistry A, 2014, 2, 19707-19716.	5.2	52
92	First-principles calculations of the thermodynamic properties of transuranium elements in a molten salt medium. Journal of the Korean Physical Society, 2014, 64, 806-812.	0.3	5
93	First principles study of oxygen reduction reaction mechanisms on N-doped graphene with a transition metal support. Electrochimica Acta, 2014, 140, 225-231.	2.6	50
94	First principles thermodynamic studies for recycling spent nuclear fuels using electrorefining with a molten salt electrolyte. Energy, 2014, 68, 751-755.	4.5	14
95	First principles computational study on the electrochemical stability of Ptâ€“Co nanocatalysts. Nanoscale, 2013, 5, 8625.	2.8	71
96	Tellurium-evaporation-annealing for p-type bismuthâ€“antimonyâ€“telluride thermoelectric materials. Journal of Alloys and Compounds, 2013, 548, 126-132.	2.8	14
97	First-principles thermodynamic study of the electrochemical stability ofÂPtÂnanoparticles in fuel cell applications. Journal of Power Sources, 2013, 238, 137-143.	4.0	40
98	The graphene-supported palladium and palladiumâ€“yttrium nanoparticles for the oxygen reduction and ethanol oxidation reactions: Experimental measurement and computational validation. Applied Catalysis B: Environmental, 2013, 129, 163-171.	10.8	86
99	First-Principles Based Analysis of the Electrocatalytic Activity of the Unreconstructed Pt(100) Surface for Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2012, 116, 6174-6183.	1.5	48
100	Structures and Formation Energies of LixC6(x=1-3) and its Homologues for Lithium Rechargeable Batteries. Bulletin of the Korean Chemical Society, 2011, 32, 2045-2050.	1.0	18
101	Electrochemical Stability of Nanometer-Scale Pt Particles in Acidic Environments. Journal of the American Chemical Society, 2010, 132, 596-600.	6.6	310
102	Electrochemical modeling of intercalation processes with phase field models. Electrochimica Acta, 2004, 49, 4691-4699.	2.6	190
103	CO2-Selective Zeolitic Imidazolate Framework Membrane on Graphene Oxide Nanoribbons: Experimental and Theoretical Studies. Journal of Materials Chemistry A, 0, , .	5.2	6