Chaozheng He

List of Publications by Year
in descending order

56 papers	2,197 citations	218677 26 h-index	233421 45 g-index
56 all docs	56 docs citations	56 times ranked	1301 citing authors

#	Article	IF	Citations
1	Graphyne as a promising substrate for the noble-metal single-atom catalysts. Carbon, 2015, 95, 756-765.	10.3	181
2	Construction of Cr-embedded graphyne electrocatalyst for highly selective reduction of CO2 to CH4: A DFT study. Chemical Engineering Journal, 2021, 414, 128857.	12.7	150
3	Highly dispersive and stable Fe³⁺ active sites on 2D graphitic carbon nitride nanosheets for efficient visible-light photocatalytic nitrogen fixation. Journal of Materials Chemistry A, 2019, 7, 27547-27559.	10.3	142
4	Synergistically boosting highly selective CO2â€“toâ€“CO photoreduction over BiOCl nanosheets via in-situ formation of surface defects and non-precious metal nanoparticles. Applied Catalysis B: Environmental, 2021, 297, 120413.	20.2	112
5	B-Doped 2D-InSe as a bifunctional catalyst for CO₂/CH₄separation under the regulation of an external electric field. Physical Chemistry Chemical Physics, 2021, 23, 23219-23224.	2.8	90
6	Capture and separation of CO2 on BC3 nanosheets: A DFT study. Chinese Chemical Letters, 2021, 32, 3202-3206.	9.0	90
7	Charge-regulated CO2 capture capacity of metal atom embedded graphyne: A first-principles study. Applied Surface Science, 2020, 509, 145392.	6.1	79
8	Density functional theory study of transition metal single-atoms anchored on graphyne as efficient electrocatalysts for the nitrogen reduction reaction. Physical Chemistry Chemical Physics, 2021, 23, 10418-10428.	2.8	68
9	Design strategies of two-dimensional metalâ€“organic frameworks toward efficient electrocatalysts for N₂ reduction: cooperativity of transition metals and organic linkers. Nanoscale, 2021, 13, 19247-19254.	5.6	67
10	Potential active sites of Mo single atoms for electrocatalytic reduction of N2. Chinese Chemical Letters, 2021, 32, 53-56.	9.0	66
11	Predicted a honeycomb metallic BiC and a direct semiconducting Bi2C monolayer as excellent CO2 adsorbents. Chinese Chemical Letters, 2022, 33, 2595-2599.	9.0	64
12	Rich B active centers in Penta-B2C as high-performance photocatalyst for nitrogen reduction. Chinese Chemical Letters, 2021, 32, 3821-3824.	9.0	63
13	Associative vs. dissociative mechanism: Electrocatalysis of nitric oxide to ammonia. Chinese Chemical Letters, 2022, 33, 1051-1057.	9.0	61
14	Computational design of BC3N2 based single atom catalyst for dramatic activation of inert CO2 and CH4 gasses into CH3COOH with ultralow CH4 dissociation barrier. Chinese Chemical Letters, 2023, 34, 107213.	9.0	61
15	Hydrogen generation of ammonia borane hydrolysis catalyzed by Fe22@Co58 core-shell structure. Chinese Chemical Letters, 2021, 32, 2269-2273.	9.0	59
16	Fe-embedded Au (111) monolayer as an electrocatalyst for N2 reduction reaction: A first-principles investigation. Journal of Alloys and Compounds, 2021, 875, 159907.	5.5	59
17	Prediction of stable BC3N2 monolayer from first-principles calculations: Stoichiometry, crystal structure, electronic and adsorption properties. Chinese Chemical Letters, 2021, 32, 3149-3154.	9.0	57
18	Defect engineering for high-selection-performance of NO reduction to NH3 over CeO2 (111) surface: A DFT study. Chinese Chemical Letters, 2022, 33, 527-532.	9.0	53

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19	A Theoretical Evaluation of Possible N₂ Reduction Mechanism on Mo₂B₂. Advanced Theory and Simulations, 2021, 4, 2100003.	2.8	49
20	Highly active Fe36Co44 bimetallic nanoclusters catalysts for hydrolysis of ammonia borane: The first-principles study. Chinese Chemical Letters, 2023, 34, 107261.	9.0	46
21	Two-dimensional 1T-PS2 as a promising anode material for sodium-ion batteries with ultra-high capacity, low average voltage and appropriate mobility. Chinese Chemical Letters, 2020, 31, 2325-2329.	9.0	42
22	Prediction of semiconducting SiP2 monolayer with negative Possionâ€™s ratio, ultrahigh carrier mobility and CO2 capture ability. Chinese Chemical Letters, 2021, 32, 1089-1094.	9.0	42
23	Electro-reduction of N2 on nanostructured materials and the design strategies of advanced catalysts based on descriptors. Materials Today Physics, 2022, 22, 100609.	6.0	42
24	First-principles study on Fe2B2 as efficient catalyst for nitrogen reduction reaction. Chinese Chemical Letters, 2021, 32, 3137-3142.	9.0	38
25	Principles for designing CO2 adsorption catalyst: Serving thermal conductivity as the determinant for reactivity. Chinese Chemical Letters, 2022, 33, 990-994.	9.0	36
26	Porous carbon framework nested nickel foam as freestanding host for high energy lithium sulfur batteries. Chinese Chemical Letters, 2021, 32, 1106-1110.	9.0	35
27	Two-dimensional MgSiP2 with anisotropic electronic properties and good performances for Na-ion batteries. Chinese Chemical Letters, 2021, 32, 1081-1085.	9.0	26
28	Carbonâ€Coordinated Single Cr Site for Efficient Electrocatalytic N₂ Fixation. Advanced Theory and Simulations, 2021, 4, 2100044.	2.8	24
29	Computational Screening of 3â€‰d Transition Metal Atoms Anchored on Defective Graphene for Efficient Electrocatalytic N₂ Fixation. ChemPhysChem, 2021, 22, 1712-1721.	2.1	22
30	The growth pattern of Ptn (nâ€¯=â€¯1â€“6) clusters on pentagonal B2C monolayer support: A computational study. Applied Surface Science, 2020, 507, 145076.	6.1	20
31	First principle investigation of W/P3C sheet as an efficient single atom electrocatalyst for N2 and NO electrochemical reaction with suppressed hydrogen evolution. Fuel, 2022, 308, 122068.	6.4	20
32	Boosting polysulfides immobilization and conversion through CoS2 catalytic sites loaded carbon fiber for robust lithium sulfur batteries. Journal of Colloid and Interface Science, 2022, 608, 963-972.	9.4	20
33	Multi-interfacial engineering of a coil-like NiSâ€“Ni₂P/Ni hybrid to efficiently boost electrocatalytic hydrogen generation in alkaline and neutral electrolyte. Journal of Materials Chemistry A, 2022, 10, 13410-13417.	10.3	16
34	Density functional theory study of a two-atom active site transition-metal/iridium electrocatalyst for ammonia synthesis. Journal of Materials Chemistry A, 2022, 10, 13946-13957.	10.3	16
35	Copper-sulfide cluster assembled architecture via in situ reaction. Chinese Chemical Letters, 2020, 31, 3213-3215.	9.0	15
36	Conversion of Dinitrogen to Ammonia by FeBâ€‘Embedded Graphyne. Journal of the Electrochemical Society, 2021, 168, 066503.	2.9	15

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37	Harnessing Adsorptionâ€“Catalysis Synergy: Efficient Oxidative Removal of Gaseous Formaldehyde by a Manganese Dioxide/Metalâ€“Organic Framework Nanocomposite at Room Temperature. Advanced Functional Materials, 2022, 32, .	14.9	15
38	Constructing a novel Ag nanowire@CeVO4 heterostructure photocatalyst for promoting charge separation and sunlight driven photodegradation of organic pollutants. Chinese Chemical Letters, 2022, 33, 1283-1287.	9.0	14
39	Adsorption and electric field assisted activation of ammonia -borane over BC3 sheet: A computational study. International Journal of Hydrogen Energy, 2022, 47, 7738-7750.	7.1	12
40	MXene-supported NiMn-LDHs as efficient electrocatalysts towards enhanced oxygen evolution reactions. Materials Advances, 2022, 3, 4359-4368.	5.4	12
41	A computational study of strained MoS2 as catalysts for the electrocatalytic nitrogen reduction reaction. Journal of Molecular Structure, 2022, 1259, 132746.	3.6	10
42	Increasing oxygen vacancies in CeO₂ nanocrystals by Ni doping and reduced graphene oxide decoration towards electrocatalytic hydrogen evolution. CrystEngComm, 2022, 24, 3369-3379.	2.6	9
43	An efficient single atom catalysts Os/P3C sheet for ammonia borane dehydrogenation. Chinese Chemical Letters, 2022, 33, 3281-3286.	9.0	8
44	First-principles study of two-dimensional material Cr2B2 as catalyst for electrochemical nitrogen reduction reaction. Journal of Electroanalytical Chemistry, 2021, 899, 115677.	3.8	7
45	Firstâ€Principles Study of 3d Transition Metal Atoms Doped Ni₁₃ Cluster as Efficient Electrocatalyst for Nitrogen Reduction Reaction. Advanced Theory and Simulations, 2021, 4, 2100353.	2.8	7
46	Metastable FeCN₂@nitrogen-doped carbon with high pseudocapacitance as an anode material for sodium ion batteries. Nanoscale, 2022, 14, 780-789.	5.6	7
47	Mechanism of complete dehydrogenation of ammonia borane in electrochemical alkaline environment. Computational Materials Science, 2022, 207, 111306.	3.0	7
48	Density functional theory study of N2 adsorption and dissociation on 3d transition metal atoms doped Ir(1 0 0) surface. Applied Surface Science, 2022, 597, 153678.	6.1	7
49	Adsorption Characteristics of Gas Molecules Adsorbed on Graphene Doped with Mn: A First Principle Study. Molecules, 2022, 27, 2315.	3.8	6
50	Electric field controlled CO2 capture and activation on BC6N monolayers: A first-principles study. Surfaces and Interfaces, 2022, 30, 101885.	3.0	6
51	Efficient electrocatalytic reduction of NO to ammonia on BC3 nanosheets. Environmental Research, 2022, 212, 113479.	7.5	6
52	Theoretical Study on V Atom Supported on N and P-Doped Defective Graphene for Electrocatalytic Nitrogen Reduction. Journal of the Electrochemical Society, 2021, 168, 116516.	2.9	5
53	A promising controllable CO2 capture and separation materials for CO2/CH4/H2 under electric field. Chinese Chemical Letters, 2023, 34, 107581.	9.0	5
54	Design of S-vacancy FeS2 as an electrocatalyst for NO reduction reaction: A DFT study. Molecular Catalysis, 2022, 524, 112327.	2.0	4

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55	The Investigation of Adsorption Behavior of Gas Molecules on FeN3-Doped Graphene. Journal of Sensors, 2022, 2022, 1-8.	1.1	2
56	Oriented external electric fields act as a â€œswitchâ€•of Pt-M/BC3N2 diatomic catalysts activate pristine ammonia borane dehydrogenation: A DFT study. Materials Today Communications, 2022, 31, 103544.	1.9	2