Xin Chen

List of Publications by Year
in descending order

83 papers	2,214 citations	236833 25 h-index	254106 43 g-index
83 all docs	83 docs citations	83 times ranked	2462 citing authors

#	Article	IF	Citations
1	Bimetallic alloys encapsulated in fullerenes as efficient oxygen reduction or oxygen evolution reaction catalysts: A density functional theory study. Journal of Alloys and Compounds, 2022, 894, 162508.	2.8	20
2	Screening of catalytic oxygen reduction reaction activity of 2, 9-dihalo-1, 10-phenanthroline metal complexes: The role of transition metals and halogen substitution. Journal of Colloid and Interface Science, 2022, 609, 130-138.	5.0	17
3	Mechanism of CO2 hydrogenation to methanol on the W-doped Rh(111) surface unveiled by first-principles calculation. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 638, 128332.	2.3	10
4	Screening of single-atom catalysts sandwiched by boron nitride sheet and graphene for oxygen reduction and oxygen evolution. Renewable Energy, 2022, 189, 502-509.	4.3	13
5	Dual-metal-organic frameworks as ultrahigh-performance bifunctional electrocatalysts for oxygen reduction and oxygen evolution. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 644, 128882.	2.3	17
6	Two-Dimensional Metalâ€"Organic Frameworks as Ultrahigh-Performance Electrocatalysts for the Fuel Cell Cathode: A First-Principles Study. Langmuir, 2022, 38, 4996-5005.	1.6	9
7	Density functional theory study of the copper phthalocyanine based metalâˆ’organic frameworks as the highly active electrocatalysts for the oxygen reduction. International Journal of Hydrogen Energy, 2022, 47, 17611-17620.	3.8	1
8	Mechanochemical-Driven Uniformly Dispersed Monatomic Feâ€"N_{<i>x</i>} Coordination in Carbon for Facilitating Efficient Oxygen Reduction Reaction. ACS Sustainable Chemistry and Engineering, 2022, 10, 7553-7563.	3.2	11
9	Enhanced oxygen reduction reaction activity by utilizing carbon nanotube intramolecular junctions. Computational and Theoretical Chemistry, 2022, 1214, 113765.	1.1	1
10	Screening of transition metal doped two-dimensional C2N (TM-C2N) as high-performance catalyst for the non-oxidative propane dehydrogenation. Molecular Catalysis, 2022, 528, 112501.	1.0	3
11	First-principles investigation of methanol synthesis from CO2 hydrogenation on Cu@Pd coreâ€"shell surface. Journal of Materials Science, 2021, 56, 3790-3803.	1.7	10
12	Ultra-smooth CsPbI2Br film via programmable crystallization process for high-efficiency inorganic perovskite solar cells. Journal of Materials Science and Technology, 2021, 66, 150-156.	5.6	12
13	Self-synergistic cobalt catalysts with symbiotic metal single-atoms and nanoparticles for efficient oxygen reduction. Journal of Materials Chemistry A, 2021, 9, 1127-1133.	5.2	21
14	Synthesis of Salicylhydrazone Probe with High Selectivity and Rapid Detection Cu2+ and Its Application in Logic Gate and Adsorption. Chinese Journal of Organic Chemistry, 2021, 41, 2839.	0.6	4
15	Mechanisms of fullerene and single-walled carbon nanotube composite as the metal-free multifunctional electrocatalyst for the oxygen reduction, oxygen evolution, and hydrogen evolution. Molecular Catalysis, 2021, 502, 111383.	1.0	16
16	Probing the catalytic activity of M-N4âˆ’xOx embedded graphene for the oxygen reduction reaction by density functional theory. Frontiers of Chemical Science and Engineering, 2021, 15, 1206-1216.	2.3	38
17	Density functional theory study of the sulfur/oxygen doped CoN4-graphene electrocatalyst for oxygen reduction reaction. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2021, 615, 126219.	2.3	15
18	High mass-specific reactivity of a defect-enriched Ru electrocatalyst for hydrogen evolution in harsh alkaline and acidic media. Science China Materials, 2021, 64, 2467-2476.	3.5	16

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19	Identification of the Active Sites of NiCo₂O₄and the Support Effect with Carbon Nanotubes for Oxygen Reduction Catalysis. Langmuir, 2021, 37, 6330-6336.	1.6	21
20	Iron-zinc bimetal embedded N-doped graphene for the oxygen reduction reaction catalysis: A density functional theory study. Diamond and Related Materials, 2021, 116, 108431.	1.8	8
21	PdZn bimetallic nanoparticles for CO2 hydrogenation to methanol: Performance and mechanism. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2021, 622, 126723.	2.3	12
22	DFT study of C2N-supported Ag3M (MÂ=ÂCu, Pd, and Pt) clusters as potential oxygen reduction reaction catalysts. Chemical Engineering Science, 2021, 239, 116642.	1.9	18
23	Theoretical study on the synthesis of methane by CO2 hydrogenation on Ni3Fe(111) surface. Journal of Natural Gas Science and Engineering, 2021, 94, 104114.	2.1	11
24	Pristine inorganic nickel oxide as desirable hole transporting material for efficient quasi two-dimensional perovskite solar cells. Journal of Power Sources, 2021, 512, 230452.	4.0	9
25	Transition metal doped graphene-like germanium carbide: Screening of high performance electrocatalysts for oxygen reduction, oxygen evolution, or hydrogen evolution. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2021, 630, 127628.	2.3	17
26	Cobaltâ€based coordination polymer as high activity electrocatalyst for oxygen reduction reaction: Catalysis by novel active site CoO 4 N 2. International Journal of Energy Research, 2020, 44, 2164-2172.	2.2	9
27	Modifications of Metal and Ligand to Modulate the Oxygen Reduction Reaction Activity of Two-Dimensional MOF Catalysts. Journal of Physical Chemistry C, 2020, 124, 1413-1420.	1.5	34
28	A Novel 2-Phenyl-1,2,3-Triazole Derived Fluorescent Probe for Recyclable Detection of Al3+ in Aqueous Medium and Its Application. Russian Journal of Bioorganic Chemistry, 2020, 46, 627-641.	0.3	3
29	DFT study of CO2 catalytic conversion by H2 over Ni13 cluster. Journal of Chemical Sciences, 2020, 132, 1.	0.7	10
30	Transition metal atom doped C2N as catalyst for the oxygen reduction reaction: A density functional theory study. International Journal of Hydrogen Energy, 2020, 45, 27202-27209.	3.8	32
31	Cotton pad-derived large-area 3D N-doped graphene-like full carbon cathode with an O-rich functional group for flexible all solid Znâ€“air batteries. Journal of Materials Chemistry A, 2020, 8, 11202-11209.	5.2	42
32	Endohedral metallofullerenes Mn@C60 (Mâ€‰=â€‰Mn, Co, Ni, Cu; nâ€‰=â€‰2â€“5) as electrocatalysts for oxygen reduction reaction: a first-principles study. Journal of Materials Science, 2020, 55, 11382-11390.	1.7	17
33	Probing the Catalytic Activity and Poisoning-Tolerance Ability of Endohedral Metallofullerene Fe_{<i>n</i>}@C₆₀ (<i>n</i> = 1â^’7) Catalysts in the Oxygen Reduction Reaction. Journal of the Electrochemical Society, 2020, 167, 024515.	1.3	6
34	Novel triphenylamine-based polyamides: Efficient preparation via benzoxazine-isocyanide-chemistry at room temperature and electrochromic properties investigation. Dyes and Pigments, 2020, 176, 108206.	2.0	17
35	Indiscrete metal/metal-N-C synergic active sites for efficient and durable oxygen electrocatalysis toward advanced Zn-air batteries. Applied Catalysis B: Environmental, 2020, 272, 118967.	10.8	110
36	N, O Co-Doped Graphene as a Potential Catalyst for the Oxygen Reduction Reaction. Journal of the Electrochemical Society, 2019, 166, F847-F851.	1.3	19

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37	Exploring the catalytic activity of metalâ€fullerene C ₅₈ M (M = Mn, Fe, Co, Ni, and Cu) toward oxygen reduction and CO oxidation by density functional theory. International Journal of Energy Research, 2019, 43, 7375.	2.2	14
38	The effect of GGA functionals on the oxygen reduction reaction catalyzed by Pt(111) and FeN4 doped graphene. Journal of Molecular Modeling, 2019, 25, 180.	0.8	6
39	DFT-based study of single transition metal atom doped g-C3N4 as alternative oxygen reduction reaction catalysts. International Journal of Hydrogen Energy, 2019, 44, 15409-15416.	3.8	99
40	N-, P-, and S-doped graphene-like carbon catalysts derived from onium salts with enhanced oxygen chemisorption for Zn-air battery cathodes. Applied Catalysis B: Environmental, 2019, 241, 442-451.	10.8	284
41	DFT study of the two dimensional metalâ€“organic frameworks X3(HITP)2 as the cathode electrocatalysts for fuel cell. Applied Surface Science, 2019, 471, 256-262.	3.1	43
42	Application of DFT Methods to Investigate Activity and Stability of Oxygen Reduction Reaction Electrocatalysts. , 2018, , 337-358.		0
43	DFT Prediction of the Catalytic Oxygen Reduction Activity and Poisoning-Tolerance Ability on a Class of Fe/S/C Catalysts. Journal of the Electrochemical Society, 2018, 165, F334-F337.	1.3	18
44	Comb-shaped polyzwitterion with surface-activity obtained <i>via N</i>-maleoyl chitosan-modified HPAM for displacement of residual oil. New Journal of Chemistry, 2018, 42, 6848-6857.	1.4	9
45	Isocyano-functionalized, 1,8-naphthalimide-based chromophore as efficient ratiometric fluorescence probe for Hg2+ in aqueous medium. Sensors and Actuators B: Chemical, 2018, 255, 3074-3084.	4.0	27
46	Probing the activity of pure and N-doped fullerenes towards oxygen reduction reaction by density functional theory. Carbon, 2018, 126, 53-57.	5.4	76
47	Particle size effect of Ag catalyst for oxygen reduction reaction: Activity and stability. Journal of Renewable and Sustainable Energy, 2018, 10, 054301.	0.8	8
48	Catalytic performance of M@Ni (M = Fe, Ru, Ir) coreâ^'shell nanoparticles towards ammonia decomposition for COx-free hydrogen production. Journal of Nanoparticle Research, 2018, 20, 1.	0.8	11
49	Transformation of H-Aggregates and J-Dimers of Water-Soluble Tetrakis (4-carboxyphenyl) Porphyrin in Polyion Complex Micelles. Polymers, 2018, 10, 494.	2.0	12
50	Cobalt or Nickel Doped SiC Nanocages as Efficient Electrocatalyst for Oxygen Reduction Reaction: A Computational Prediction. Journal of the Electrochemical Society, 2017, 164, F616-F619.	1.3	47
51	Soluble graphene composite with aggregation-induced emission feature: non-covalent functionalization and application in explosive detection. Journal of Materials Chemistry C, 2017, 5, 6216-6223.	2.7	18
52	Oxygen reduction reaction on Ni 3 (HITP) 2 : A catalytic site that leads to high activity. Electrochemistry Communications, 2017, 82, 89-92.	2.3	50
53	Nanoscale size effect of octahedral nickel catalyst towards ammonia decomposition reaction. International Journal of Hydrogen Energy, 2017, 42, 17122-17128.	3.8	14
54	Probing the activity of Ni13, Cu13, and Ni12Cu clusters towards the ammonia decomposition reaction by density functional theory. Journal of Materials Science, 2017, 52, 3162-3168.	1.7	17

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55	DFT Study of the Oxygen Reduction Reaction Activity on Feâˆ'N4-Patched Carbon Nanotubes: The Influence of the Diameter and Length. Materials, 2017, 10, 549.	1.3	18
56	Germanium Nanotube as the Catalyst for Oxygen Reduction Reaction: Performance and Mechanism. Acta Chimica Sinica, 2017, 75, 189.	0.5	1
57	Adsorption of naphthenic acids to the nitrogen-coordinated transition-metal embedded graphene: A DFT study. Russian Journal of Physical Chemistry B, 2016, 10, 1027-1031.	0.2	8
58	Boron Nitride Nanocages as High Activity Electrocatalysts for Oxygen Reduction Reaction: Synergistic Catalysis by Dual Active Sites. Journal of Physical Chemistry C, 2016, 120, 28912-28916.	1.5	41
59	An aggregation-induced emission enhancement fluorescent benzoxazine-derived macromolecule: catalyst-free synthesis and its preliminary application for the determination of aqueous picric acid. RSC Advances, 2016, 6, 41340-41347.	1.7	10
60	Screening of catalytic oxygen reduction reaction activity of metal-doped graphene by density functional theory. Applied Surface Science, 2016, 379, 291-295.	3.1	81
61	The role of chelating ligands and central metals in the oxygen reduction reaction activity: a DFT study. Russian Journal of Electrochemistry, 2016, 52, 555-559.	0.3	2
62	A comparative DFT study of oxygen reduction reaction on mononuclear and binuclear cobalt and iron phthalocyanines. Russian Journal of Physical Chemistry A, 2016, 90, 2413-2417.	0.1	14
63	Benzylidenecyclohexanone-triazole-based conjugated polymer: Click synthesis, Staudinger end-capping and application as optical probe scaffold. Dyes and Pigments, 2016, 133, 406-414.	2.0	4
64	Oxygen reduction reaction on cobaltâ€"(n)pyrrole clusters from DFT studies. RSC Advances, 2016, 6, 5535-5540.	1.7	9
65	Simple-structured, hydrazinecarbothioamide derivatived dual-channel optical probe for Hg2+ and Ag+. Journal of Luminescence, 2016, 174, 56-62.	1.5	39
66	Catalytic performance and mechanism of N-CoTi@CoTiO 3 catalysts for oxygen reduction reaction. Nano Energy, 2016, 20, 134-143.	8.2	33
67	Diphenylphosphorylâ€Triazoleâ€Tethered, AIEEâ€Type Conjugated Polymer as Optical Probe for Silver Ion in Relatively Highâ€Waterâ€Fraction Medium. Macromolecular Chemistry and Physics, 2015, 216, 2263-2269.	1.1	4
68	Origins for the Synergetic Effects of AuCu₃ in Catalysis for Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2015, 119, 907-912.	1.5	13
69	Enhanced electrocatalytic performance for methanol oxidation with a MagnÃ©li phase molybdenum oxide/Pt-black composite. Journal of Molecular Catalysis A, 2015, 400, 7-13.	4.8	12
70	Why Do Boron and Nitrogen Doped Î±- and Î³-Graphyne Exhibit Different Oxygen Reduction Mechanism? A First-Principles Study. Journal of Physical Chemistry C, 2015, 119, 11493-11498.	1.5	77
71	Graphyne nanotubes as electrocatalysts for oxygen reduction reaction: the effect of doping elements on the catalytic mechanisms. Physical Chemistry Chemical Physics, 2015, 17, 29340-29343.	1.3	62
72	Theoretical evaluation of corrosion inhibition performance of three antipyrine compounds. Computational and Theoretical Chemistry, 2015, 1072, 7-14.	1.1	95

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73	Electrocatalytic Dechlorination of Atrazine Using Binuclear Iron Phthalocyanine as Electrocatalysts. Electrocatalysis, 2014, 5, 68-74.	1.5	20
74	Nanoâ€Intermetallic AuCu₃ Catalyst for Oxygen Reduction Reaction: Performance and Mechanism. Small, 2014, 10, 2662-2669.	5.2	54
75	A novel CoN electrocatalyst with high activity and stability toward oxygen reduction reaction. Journal of Materials Chemistry A, 2014, 2, 62-65.	5.2	55
76	Mechanism of oxygen reduction reaction catalyzed by Fe(Co)â€“Nx/C. Physical Chemistry Chemical Physics, 2013, 15, 19330.	1.3	55
77	The Interactions of Oxygen with Small Gold Clusters on Nitrogen-Doped Graphene. Molecules, 2013, 18, 3279-3291.	1.7	17
78	Durability Enhancement of Intermetallics Electrocatalysts via N-anchor Effect for Fuel Cells. Scientific Reports, 2013, 3, 3234.	1.6	29
79	Density Functional Theory Study of the Oxygen Reduction Reaction on a Cobaltâ€“Polypyrrole Composite Catalyst. Journal of Physical Chemistry C, 2012, 116, 12553-12558.	1.5	35
80	DFT Study of Polyaniline and Metal Composites as Nonprecious Metal Catalysts for Oxygen Reduction in Fuel Cells. Journal of Physical Chemistry C, 2012, 116, 22737-22742.	1.5	39
81	What Differs on the Enzymatic Acetylation Mechanisms for Arylamines and Arylhydrazines Substrates? A Theoretical Study. Research Letters in Biochemistry, 2009, 2009, 1-5.	0.0	0
82	Investigation on the Scavenging Mechanism of 1,4â€Dicarbonyls by Pyridoxamine: A Density Functional Theory Study. Chinese Journal of Chemistry, 2009, 27, 1452-1458.	2.6	1
83	Theoretical study of the scavenging mechanism to 1,4-dicarbonyls by pyridoxamine: The water-assisted reaction. Computational and Theoretical Chemistry, 2009, 911, 70-74.	1.5	4