Xin Chen

List of Publications by Year
in descending order

83	2,214	25	43
papers	citations	h-index	g-index
		236833	254106

83	83	83	2462
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	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
3	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
4	Theoretical evaluation of corrosion inhibition performance of three antipyrine compounds. Computational and Theoretical Chemistry, 2015, 1072, 7-14.	1.1	95
5	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
6	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
7	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
8	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
9	Mechanism of oxygen reduction reaction catalyzed by Fe(Co)â€“Nx/C. Physical Chemistry Chemical Physics, 2013, 15, 19330.	1.3	55
10	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
11	Nanoâ€Intermetallic AuCu₃ Catalyst for Oxygen Reduction Reaction: Performance and Mechanism. Small, 2014, 10, 2662-2669.	5.2	54
12	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
13	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
14	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
15	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
16	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
17	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
18	Simple-structured, hydrazinecarbothioamide derivatived dual-channel optical probe for Hg2+ and Ag+. Journal of Luminescence, 2016, 174, 56-62.	1.5	39

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19	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
20	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
21	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
22	Catalytic performance and mechanism of N-CoTi@CoTiO 3 catalysts for oxygen reduction reaction. Nano Energy, 2016, 20, 134-143.	8.2	33
23	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
24	Durability Enhancement of Intermetallics Electrocatalysts via N-anchor Effect for Fuel Cells. Scientific Reports, 2013, 3, 3234.	1.6	29
25	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
26	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
27	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
28	Electrocatalytic Dechlorination of Atrazine Using Binuclear Iron Phthalocyanine as Electrocatalysts. Electrocatalysis, 2014, 5, 68-74.	1.5	20
29	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
30	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
31	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
32	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
33	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
34	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
35	The Interactions of Oxygen with Small Gold Clusters on Nitrogen-Doped Graphene. Molecules, 2013, 18, 3279-3291.	1.7	17
36	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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37	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
38	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
39	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
40	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
41	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
42	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
43	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
44	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
45	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
46	Nanoscale size effect of octahedral nickel catalyst towards ammonia decomposition reaction. International Journal of Hydrogen Energy, 2017, 42, 17122-17128.	3.8	14
47	Exploring the catalytic activity of metalâ€ƒfullerene 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
48	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
49	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
50	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
51	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
52	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
53	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
54	Catalytic performance of M@Ni (M = Fe, Ru, Ir) coreâˆ’shell nanoparticles towards ammonia decomposition for COx-free hydrogen production. Journal of Nanoparticle Research, 2018, 20, 1.	0.8	11

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55	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
56	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
57	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
58	DFT study of CO2 catalytic conversion by H2 over Ni13 cluster. Journal of Chemical Sciences, 2020, 132, 1.	0.7	10
59	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
60	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
61	Oxygen reduction reaction on cobaltâ€“(n)pyrrole clusters from DFT studies. RSC Advances, 2016, 6, 5535-5540.	1.7	9
62	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
63	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
64	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
65	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
66	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
67	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
68	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
69	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
70	Probing the Catalytic Activity and Poisoning-Tolerance Ability of Endohedral Metallofullerene Fe_{<i>n</i>}@C₆₀ (<i>n</i> = 1âˆ'7) Catalysts in the Oxygen Reduction Reaction. Journal of the Electrochemical Society, 2020, 167, 024515.	1.3	6
71	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
72	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

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73	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
74	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
75	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
76	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
77	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
78	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
79	Germanium Nanotube as the Catalyst for Oxygen Reduction Reaction: Performance and Mechanism. Acta Chimica Sinica, 2017, 75, 189.	0.5	1
80	Density functional theory study of the copper phthalocyanine based metalâ˘organic frameworks as the highly active electrocatalysts for the oxygen reduction. International Journal of Hydrogen Energy, 2022, 47, 17611-17620.	3.8	1
81	Enhanced oxygen reduction reaction activity by utilizing carbon nanotube intramolecular junctions. Computational and Theoretical Chemistry, 2022, 1214, 113765.	1.1	1
82	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
83	Application of DFT Methods to Investigate Activity and Stability of Oxygen Reduction Reaction Electrocatalysts. , 2018, , 337-358.		0