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List of Publications by Year
in descending order

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78	5,094	101543	88630
papers	citations	36	70
		h-index	g-index

79	79	79	6720
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Revealing the intrinsic relation between heteroatom dopants and graphene quantum dots as a bi-functional ORR/OER catalyst. Molecular Catalysis, 2022, 518, 112109.	2.0	4
2	Revealing the role of HBr in propane dehydrogenation on CeO₂(111) via DFT-based microkinetic simulation. Physical Chemistry Chemical Physics, 2022, 24, 9718-9726.	2.8	3
3	Boosting acidic water oxidation performance by constructing arrays-like nanoporous IrxRu1â^'xO2 with abundant atomic steps. Nano Research, 2022, 15, 5933-5939.	10.4	25
4	A critical evaluation of the catalytic role of CO₂ in propane dehydrogenation catalyzed by chromium oxide from a DFT-based microkinetic simulation. Physical Chemistry Chemical Physics, 2022, 24, 11030-11038.	2.8	3
5	Iridiumâ€“Iron Diatomic Active Sites for Efficient Bifunctional Oxygen Electrocatalysis. ACS Catalysis, 2022, 12, 9397-9409.	11.2	47
6	Catalytic Property and Stability of Subnanometer Pt Cluster on Carbon Nanotube in Direct Propane Dehydrogenation. Chinese Journal of Chemistry, 2021, 39, 661-665.	4.9	11
7	Atomic-Step Enriched Rutheniumâ€“Iridium Nanocrystals Anchored Homogeneously on MOF-Derived Support for Efficient and Stable Oxygen Evolution in Acidic and Neutral Media. ACS Catalysis, 2021, 11, 3402-3413.	11.2	87
8	Boosting electrocatalytic activity for CO2 reduction on nitrogen-doped carbon catalysts by co-doping with phosphorus. Journal of Energy Chemistry, 2021, 54, 143-150.	12.9	43
9	Revealing nature of active site and reaction mechanism of supported chromium oxide catalyst in propane direct dehydrogenation. Molecular Catalysis, 2021, 505, 111520.	2.0	5
10	Density Functional Theory Study of a Graphdiyne-Supported Single Au Atom Catalyst for Highly Efficient Acetylene Hydrochlorination. ACS Applied Nano Materials, 2021, 4, 6152-6159.	5.0	22
11	An in-situ solidification strategy to block polysulfides in Lithium-Sulfur batteries. Energy Storage Materials, 2021, 37, 224-232.	18.0	55
12	Coke Deposition on Pt-Based Catalysts in Propane Direct Dehydrogenation: Kinetics, Suppression, and Elimination. ACS Catalysis, 2021, 11, 9279-9292.	11.2	69
13	Machine Learning Derived Blueprint for Rational Design of the Effective Single-Atom Cathode Catalyst of the Lithiumâ€“Sulfur Battery. Journal of Physical Chemistry Letters, 2021, 12, 7053-7059.	4.6	28
14	Probing the reaction mechanism of acetylene hydrochlorination on metal-free doped boron nitride: Decisive role of carbon dopant. Applied Surface Science, 2021, 566, 150710.	6.1	1
15	Self-healing effect of graphene@PANI loaded with benzotriazole for carbon steel. Corrosion Science, 2020, 163, 108246.	6.6	68
16	Robust Ruthenium-Saving Catalyst for High-Temperature Carbon Dioxide Reforming of Methane. ACS Catalysis, 2020, 10, 783-791.	11.2	45
17	Revealing the role of nitrogen dopants in tuning the electronic and optical properties of graphene quantum dots via a TD-DFT study. Physical Chemistry Chemical Physics, 2020, 22, 28230-28237.	2.8	17
18	Resolving the Mechanism Complexity of Oxidative Dehydrogenation of Hydrocarbons on Nanocarbon by Microkinetic Modeling. ACS Catalysis, 2020, 10, 14006-14014.	11.2	9

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19	Oneâ€Step Synthesis of N/S Codoped â€œPorous Carbon Clothâ€•as a Sulfur Carrier for Lithiumâ€“Sulfur Batteries. Energy Technology, 2020, 8, 2000188.	3.8	11
20	Tuning of interactions between cathode and lithium polysulfide in Li-S battery by rational halogenation. Journal of Energy Chemistry, 2020, 49, 147-152.	12.9	19
21	Strong Electronic Coupling between Ultrafine Iridiumâ€“Ruthenium Nanoclusters and Conductive, Acid-Stable Tellurium Nanoparticle Support for Efficient and Durable Oxygen Evolution in Acidic and Neutral Media. ACS Catalysis, 2020, 10, 3571-3579.	11.2	122
22	Critical Role of Interfacial Sites between Nickel and CeO₂ Support in Dry Reforming of Methane: Revisit of Reaction Mechanism and Origin of Stability. Journal of Physical Chemistry C, 2020, 124, 5118-5124.	3.1	36
23	Revealing the origin of the reactivity of metal-free boron nitride catalysts in oxidative dehydrogenation of propane. Applied Surface Science, 2020, 519, 146241.	6.1	18
24	Single Au Anion Can Catalyze Acetylene Hydrochlorination: Tunable Catalytic Performance from Rational Doping. Journal of Physical Chemistry C, 2019, 123, 29203-29208.	3.1	26
25	The origin of the extraordinary stability of mercury catalysts on the carbon support: the synergy effects between oxygen groups and defects revealed from a combined experimental and DFT study. Chinese Journal of Catalysis, 2019, 40, 141-146.	14.0	23
26	Wet-Chemistry Strong Metalâ€“Support Interactions in Titania-Supported Au Catalysts. Journal of the American Chemical Society, 2019, 141, 2975-2983.	13.7	280
27	Defect-rich activated carbons as active and stable metal-free catalyst for acetylene hydrochlorination. Carbon, 2019, 146, 406-412.	10.3	78
28	Screening of active center and reactivity descriptor in acetylene hydrochlorination on metal-free doped carbon catalysts from first principle calculations. Applied Surface Science, 2019, 478, 574-580.	6.1	21
29	Electronic interaction between single Pt atom and vacancies on boron nitride nanosheets and its influence on the catalytic performance in the direct dehydrogenation of propane. Chinese Journal of Catalysis, 2019, 40, 819-825.	14.0	25
30	A Deoximation Method for Deprotection of Ketones and Aldhydes Using a Grapheneâ€Oxideâ€Based Coâ€catalysts System. Advanced Synthesis and Catalysis, 2019, 361, 3137-3145.	4.3	10
31	Halogenation of graphene triggered by heteroatom doping. RSC Advances, 2019, 9, 37507-37511.	3.6	10
32	The stability and reactivity of transition metal atoms supported mono and di vacancies defected carbon based materials revealed from first principles study. Applied Surface Science, 2019, 473, 777-784.	6.1	30
33	Cyano group modified carbon nitride with enhanced photoactivity for selective oxidation of benzylamine. Applied Catalysis B: Environmental, 2019, 242, 67-75.	20.2	87
34	Revealing the Janus Character of the Coke Precursor in the Propane Direct Dehydrogenation on Pt Catalysts from a kMC Simulation. ACS Catalysis, 2018, 8, 4694-4704.	11.2	85
35	Boosting the hydrogen evolution performance of ruthenium clusters through synergistic coupling with cobalt phosphide. Energy and Environmental Science, 2018, 11, 1819-1827.	30.8	350
36	Ionâ€“Solvent Complexes Promote Gas Evolution from Electrolytes on a Sodium Metal Anode. Angewandte Chemie, 2018, 130, 742-745.	2.0	35

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37	Oxidative dehydrogenation reaction of short alkanes on nanostructured carbon catalysts: a computational account. Chemical Communications, 2018, 54, 864-875.	4.1	30
38	Tunable Catalytic Performance of Single Pt Atom on Doped Graphene in Direct Dehydrogenation of Propane by Rational Doping: A Density Functional Theory Study. Journal of Physical Chemistry C, 2018, 122, 1570-1576.	3.1	52
39	Ti₃C₂T_x MXene Catalyzed Ethylbenzene Dehydrogenation: Active Sites and Mechanism Exploration from both Experimental and Theoretical Aspects. ACS Catalysis, 2018, 8, 10051-10057.	11.2	79
40	DFT study on the active site of the monometric molybdenum anchored on silica for the selective oxidation of ethane to acetaldehyde. Molecular Catalysis, 2018, 460, 83-86.	2.0	3
41	Phosphorus-doped onion-like carbon for CO₂ electrochemical reduction: the decisive role of the bonding configuration of phosphorus. Journal of Materials Chemistry A, 2018, 6, 19998-20004.	10.3	51
42	Ionâ€“Solvent Complexes Promote Gas Evolution from Electrolytes on a Sodium Metal Anode. Angewandte Chemie - International Edition, 2018, 57, 734-737.	13.8	208
43	Towards stable lithium-sulfur batteries: Mechanistic insights into electrolyte decomposition on lithium metal anode. Energy Storage Materials, 2017, 8, 194-201.	18.0	171
44	An Analogous Periodic Law for Strong Anchoring of Polysulfides on Polar Hosts in Lithium Sulfur Batteries: S- or Li-Binding on First-Row Transition-Metal Sulfides?. ACS Energy Letters, 2017, 2, 795-801.	17.4	264
45	Revealing the Role of sp²@sp³ Structure of Nanodiamond in Direct Dehydrogenation: Insight from DFT study. ACS Catalysis, 2017, 7, 3779-3785.	11.2	29
46	The synergy effect and reaction pathway in the oxygen reduction reaction on the sulfur and nitrogen dual doped graphene catalyst. Chemical Physics Letters, 2017, 677, 65-69.	2.6	29
47	CO₂electoreduction reaction on heteroatom-doped carbon cathode materials. Journal of Materials Chemistry A, 2017, 5, 21596-21603.	10.3	60
48	The tunable effect of nitrogen and boron dopants on a single walled carbon nanotube support on the catalytic properties of a single gold atom catalyst: a first principles study of CO oxidation. Journal of Materials Chemistry A, 2017, 5, 16653-16662.	10.3	58
49	The effect of defects on the catalytic activity of single Au atom supported carbon nanotubes and reaction mechanism for CO oxidation. Physical Chemistry Chemical Physics, 2017, 19, 22344-22354.	2.8	38
50	Design Principles for Heteroatom-Doped Nanocarbon to Achieve Strong Anchoring of Polysulfides for Lithium-Sulfur Batteries. Small, 2016, 12, 3283-3291.	10.0	661
51	Designing graphene as a new frustrated Lewis pair catalyst for hydrogen activation by co-doping. Physical Chemistry Chemical Physics, 2016, 18, 11120-11124.	2.8	46
52	The Unexpected Reactivity of the Carbon Sites on the Nanostructured Carbon Catalysts towards the Câ^'H Bond Activation from the Analysis of the Aromaticity. Chemistry - an Asian Journal, 2016, 11, 1668-1671.	3.3	10
53	Hierarchical Nitrogenâ€Doped Graphene/Carbon Nanotube Composite Cathode for Lithiumâ€“Oxygen Batteries. ChemSusChem, 2015, 8, 3973-3976.	6.8	50
54	Active Sites and Mechanisms for Direct Oxidation of Benzene to Phenol over Carbon Catalysts. Angewandte Chemie - International Edition, 2015, 54, 4105-4109.	13.8	115

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55	The formation of strong-couple interactions between nitrogen-doped graphene and sulfur/lithium (poly)sulfides in lithium-sulfur batteries. 2D Materials, 2015, 2, 014011.	4.4	94
56	Calibration of the basic strength of the nitrogen groups on the nanostructured carbon materials. Physical Chemistry Chemical Physics, 2015, 17, 6691-6694.	2.8	105
57	Rationale of the effects from dopants on Câ€“H bond activation for sp²hybridized nanostructured carbon catalysts. Nanoscale, 2015, 7, 16597-16600.	5.6	13
58	Efficient Metal-Free Catalytic Reaction Pathway for Selective Oxidation of Substituted Phenols. ACS Catalysis, 2015, 5, 5921-5926.	11.2	31
59	The Nucleophilicity of the Oxygen Functional Groups on Carbon Materials: A DFT Analysis. Chemistry - A European Journal, 2014, 20, 7890-7894.	3.3	46
60	Selective Hydrogenation of Cinnamaldehyde to Cinnamal Alcohol over Platinum/Graphene Catalysts. ChemCatChem, 2014, 6, 3246-3253.	3.7	80
61	The first principles studies on the reaction pathway of the oxidative dehydrogenation of ethane on the undoped and doped carbon catalyst. Journal of Materials Chemistry A, 2014, 2, 5287.	10.3	45
62	Revealing the nature of the active site on the carbon catalyst for Câ€“H bond activation. Chemical Communications, 2014, 50, 11016-11019.	4.1	19
63	Insight into the mechanism of nanodiamond catalysed decomposition of methane molecules. Physical Chemistry Chemical Physics, 2014, 16, 4488-4491.	2.8	21
64	The Catalytic Pathways of Hydrohalogenation over Metalâ€Free Nitrogenâ€Doped Carbon Nanotubes. ChemSusChem, 2014, 7, 723-728.	6.8	114
65	Theoretical Studies on Ethylene Selectivity in the Oxidative Dehydrogenation Reaction on Undoped and Doped Nanostructured Carbon Catalysts. Chemistry - an Asian Journal, 2013, 8, 2605-2608.	3.3	18
66	First-Principles Studies of the Activation of Oxygen Molecule and Its Role in Partial Oxidation of Methane on Boron-Doped Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2013, 117, 17485-17492.	3.1	17
67	Ethane Activation by Nb-Doped NiO. Journal of Physical Chemistry C, 2013, 117, 23597-23608.	3.1	26
68	Methane Oxidation by Lanthanum Oxide Doped with Cu, Zn, Mg, Fe, Nb, Ti, Zr, or Ta: The Connection Between the Activation Energy and the Energy of Oxygen-Vacancy Formation. Catalysis Letters, 2013, 143, 406-410.	2.6	37
69	Methane Dissociation on Li-, Na-, K-, and Cu-Doped Flat and Stepped CaO(001). Journal of Physical Chemistry C, 2013, 117, 7114-7122.	3.1	24
70	Does Halogen Adsorption Activate the Oxygen Atom on an Oxide Surface? I. A Study of Br₂ and HBr Adsorption on La₂O₃ and La₂O₃ Doped with Mg or Zr. Journal of Physical Chemistry C, 2012, 116, 4137-4148.	3.1	20
71	Chemistry of Lewis Acidâ€“Base Pairs on Oxide Surfaces. Journal of Physical Chemistry C, 2012, 116, 10439-10450.	3.1	293
72	Dissociation of Methane on La₂O₃ Surfaces Doped with Cu, Mg, or Zn. Journal of Physical Chemistry C, 2011, 115, 18239-18246.	3.1	31

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73	Chemistry of Doped Oxides: The Activation of Surface Oxygen and the Chemical Compensation Effect. Journal of Physical Chemistry C, 2011, 115, 3065-3074.	3.1	102
74	DFT Studies of Oxygen Vacancies on Undoped and Doped La₂O₃ Surfaces. Journal of Physical Chemistry C, 2010, 114, 12234-12244.	3.1	101
75	How strong is the bond between water and salt?. Surface Science, 2008, 602, L135-L138.	1.9	21
76	Density functional theory study of flat and stepped NaCl(001). Physical Review B, 2007, 76, .	3.2	40
77	â€œTextbookâ€•Adsorption at â€œNontextbookâ€•Adsorption Sites: Halogen Atoms on Alkali Halide Surfaces. Physical Review Letters, 2006, 97, 046802.	7.8	10
78	Theoretical studies on dynamics and thermochemistry of the reactions CF3CHCl2+Clâ†'CF3CCl2+HCl and CF3CHFCl+Clâ†'CF3CFCl+HCl. Journal of Chemical Physics, 2004, 120, 6019-6027.	3.0	5