

Bo Li

List of Publications by Year in descending order

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101543

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#	ARTICLE	IF	CITATIONS
1	Design Principles for Heteroatom-Doped Nanocarbon to Achieve Strong Anchoring of Polysulfides for Lithium-Sulfur Batteries. <i>Small</i> , 2016, 12, 3283-3291.	10.0	661
2	Boosting the hydrogen evolution performance of ruthenium clusters through synergistic coupling with cobalt phosphide. <i>Energy and Environmental Science</i> , 2018, 11, 1819-1827.	30.8	350
3	Chemistry of Lewis Acid-Base Pairs on Oxide Surfaces. <i>Journal of Physical Chemistry C</i> , 2012, 116, 10439-10450.	3.1	293
4	Wet-Chemistry Strong Metal-Support Interactions in Titania-Supported Au Catalysts. <i>Journal of the American Chemical Society</i> , 2019, 141, 2975-2983.	13.7	280
5	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?. <i>ACS Energy Letters</i> , 2017, 2, 795-801.	17.4	264
6	Ion-Solvent Complexes Promote Gas Evolution from Electrolytes on a Sodium Metal Anode. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 734-737.	13.8	208
7	Towards stable lithium-sulfur batteries: Mechanistic insights into electrolyte decomposition on lithium metal anode. <i>Energy Storage Materials</i> , 2017, 8, 194-201.	18.0	171
8	Strong Electronic Coupling between Ultrafine Iridium-Ruthenium Nanoclusters and Conductive, Acid-Stable Tellurium Nanoparticle Support for Efficient and Durable Oxygen Evolution in Acidic and Neutral Media. <i>ACS Catalysis</i> , 2020, 10, 3571-3579.	11.2	122
9	Active Sites and Mechanisms for Direct Oxidation of Benzene to Phenol over Carbon Catalysts. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 4105-4109.	13.8	115
10	The Catalytic Pathways of Hydrohalogenation over Metal-Free Nitrogen-Doped Carbon Nanotubes. <i>ChemSusChem</i> , 2014, 7, 723-728.	6.8	114
11	Calibration of the basic strength of the nitrogen groups on the nanostructured carbon materials. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 6691-6694.	2.8	105
12	Chemistry of Doped Oxides: The Activation of Surface Oxygen and the Chemical Compensation Effect. <i>Journal of Physical Chemistry C</i> , 2011, 115, 3065-3074.	3.1	102
13	DFT Studies of Oxygen Vacancies on Undoped and Doped $\text{La}_{2}\text{O}_{3}$ Surfaces. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12234-12244.	3.1	101
14	The formation of strong-couple interactions between nitrogen-doped graphene and sulfur/lithium (poly)sulfides in lithium-sulfur batteries. <i>2D Materials</i> , 2015, 2, 014011.	4.4	94
15	Cyano group modified carbon nitride with enhanced photoactivity for selective oxidation of benzylamine. <i>Applied Catalysis B: Environmental</i> , 2019, 242, 67-75.	20.2	87
16	Atomic-Step Enriched Ruthenium-Iridium Nanocrystals Anchored Homogeneously on MOF-Derived Support for Efficient and Stable Oxygen Evolution in Acidic and Neutral Media. <i>ACS Catalysis</i> , 2021, 11, 3402-3413.	11.2	87
17	Revealing the Janus Character of the Coke Precursor in the Propane Direct Dehydrogenation on Pt Catalysts from a kMC Simulation. <i>ACS Catalysis</i> , 2018, 8, 4694-4704.	11.2	85
18	Selective Hydrogenation of Cinnamaldehyde to Cinnamal Alcohol over Platinum/Graphene Catalysts. <i>ChemCatChem</i> , 2014, 6, 3246-3253.	3.7	80

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19	Ti ₃ C ₂ T _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
20	Defect-rich activated carbons as active and stable metal-free catalyst for acetylene hydrochlorination. Carbon, 2019, 146, 406-412.	10.3	78
21	Coke Deposition on Pt-Based Catalysts in Propane Direct Dehydrogenation: Kinetics, Suppression, and Elimination. ACS Catalysis, 2021, 11, 9279-9292.	11.2	69
22	Self-healing effect of graphene@PANI loaded with benzotriazole for carbon steel. Corrosion Science, 2020, 163, 108246.	6.6	68
23	CO ₂ electroreduction reaction on heteroatom-doped carbon cathode materials. Journal of Materials Chemistry A, 2017, 5, 21596-21603.	10.3	60
24	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
25	An in-situ solidification strategy to block polysulfides in Lithium-Sulfur batteries. Energy Storage Materials, 2021, 37, 224-232.	18.0	55
26	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
27	Phosphorus-doped onion-like carbon for CO ₂ electrochemical reduction: the decisive role of the bonding configuration of phosphorus. Journal of Materials Chemistry A, 2018, 6, 19998-20004.	10.3	51
28	Hierarchical Nitrogen-Doped Graphene/Carbon Nanotube Composite Cathode for Lithium-Oxygen Batteries. ChemSusChem, 2015, 8, 3973-3976.	6.8	50
29	Iridium-Iron Diatomic Active Sites for Efficient Bifunctional Oxygen Electrocatalysis. ACS Catalysis, 2022, 12, 9397-9409.	11.2	47
30	The Nucleophilicity of the Oxygen Functional Groups on Carbon Materials: A DFT Analysis. Chemistry - A European Journal, 2014, 20, 7890-7894.	3.3	46
31	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
32	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
33	Robust Ruthenium-Saving Catalyst for High-Temperature Carbon Dioxide Reforming of Methane. ACS Catalysis, 2020, 10, 783-791.	11.2	45
34	Boosting electrocatalytic activity for CO ₂ reduction on nitrogen-doped carbon catalysts by co-doping with phosphorus. Journal of Energy Chemistry, 2021, 54, 143-150.	12.9	43
35	Density functional theory study of flat and stepped NaCl(001). Physical Review B, 2007, 76, .	3.2	40
36	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

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37	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. <i>Catalysis Letters</i> , 2013, 143, 406-410.	2.6	37
38	Critical Role of Interfacial Sites between Nickel and CeO ₂ Support in Dry Reforming of Methane: Revisit of Reaction Mechanism and Origin of Stability. <i>Journal of Physical Chemistry C</i> , 2020, 124, 5118-5124.	3.1	36
39	Ion-Solvent Complexes Promote Gas Evolution from Electrolytes on a Sodium Metal Anode. <i>Angewandte Chemie</i> , 2018, 130, 742-745.	2.0	35
40	Dissociation of Methane on La ₂ O ₃ Surfaces Doped with Cu, Mg, or Zn. <i>Journal of Physical Chemistry C</i> , 2011, 115, 18239-18246.	3.1	31
41	Efficient Metal-Free Catalytic Reaction Pathway for Selective Oxidation of Substituted Phenols. <i>ACS Catalysis</i> , 2015, 5, 5921-5926.	11.2	31
42	Oxidative dehydrogenation reaction of short alkanes on nanostructured carbon catalysts: a computational account. <i>Chemical Communications</i> , 2018, 54, 864-875.	4.1	30
43	The stability and reactivity of transition metal atoms supported mono and di vacancies defected carbon based materials revealed from first principles study. <i>Applied Surface Science</i> , 2019, 473, 777-784.	6.1	30
44	Revealing the Role of sp ² @sp ³ Structure of Nanodiamond in Direct Dehydrogenation: Insight from DFT study. <i>ACS Catalysis</i> , 2017, 7, 3779-3785.	11.2	29
45	The synergy effect and reaction pathway in the oxygen reduction reaction on the sulfur and nitrogen dual doped graphene catalyst. <i>Chemical Physics Letters</i> , 2017, 677, 65-69.	2.6	29
46	Machine Learning Derived Blueprint for Rational Design of the Effective Single-Atom Cathode Catalyst of the Lithium-Sulfur Battery. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 7053-7059.	4.6	28
47	Ethane Activation by Nb-Doped NiO. <i>Journal of Physical Chemistry C</i> , 2013, 117, 23597-23608.	3.1	26
48	Single Au Anion Can Catalyze Acetylene Hydrochlorination: Tunable Catalytic Performance from Rational Doping. <i>Journal of Physical Chemistry C</i> , 2019, 123, 29203-29208.	3.1	26
49	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. <i>Chinese Journal of Catalysis</i> , 2019, 40, 819-825.	14.0	25
50	Boosting acidic water oxidation performance by constructing arrays-like nanoporous Ir _x Ru _{1-x} O ₂ with abundant atomic steps. <i>Nano Research</i> , 2022, 15, 5933-5939.	10.4	25
51	Methane Dissociation on Li-, Na-, K-, and Cu-Doped Flat and Stepped CaO(001). <i>Journal of Physical Chemistry C</i> , 2013, 117, 7114-7122.	3.1	24
52	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. <i>Chinese Journal of Catalysis</i> , 2019, 40, 141-146.	14.0	23
53	Density Functional Theory Study of a Graphdiyne-Supported Single Au Atom Catalyst for Highly Efficient Acetylene Hydrochlorination. <i>ACS Applied Nano Materials</i> , 2021, 4, 6152-6159.	5.0	22
54	How strong is the bond between water and salt?. <i>Surface Science</i> , 2008, 602, L135-L138.	1.9	21

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55	Insight into the mechanism of nanodiamond catalysed decomposition of methane molecules. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4488-4491.	2.8	21
56	Screening of active center and reactivity descriptor in acetylene hydrochlorination on metal-free doped carbon catalysts from first principle calculations. <i>Applied Surface Science</i> , 2019, 478, 574-580.	6.1	21
57	Does Halogen Adsorption Activate the Oxygen Atom on an Oxide Surface? I. A Study of Br ₂ and HBr Adsorption on La ₂ O ₃ and La ₂ O ₃ Doped with Mg or Zr. <i>Journal of Physical Chemistry C</i> , 2012, 116, 4137-4148.	3.1	20
58	Revealing the nature of the active site on the carbon catalyst for C-H bond activation. <i>Chemical Communications</i> , 2014, 50, 11016-11019.	4.1	19
59	Tuning of interactions between cathode and lithium polysulfide in Li-S battery by rational halogenation. <i>Journal of Energy Chemistry</i> , 2020, 49, 147-152.	12.9	19
60	Theoretical Studies on Ethylene Selectivity in the Oxidative Dehydrogenation Reaction on Undoped and Doped Nanostructured Carbon Catalysts. <i>Chemistry - an Asian Journal</i> , 2013, 8, 2605-2608.	3.3	18
61	Revealing the origin of the reactivity of metal-free boron nitride catalysts in oxidative dehydrogenation of propane. <i>Applied Surface Science</i> , 2020, 519, 146241.	6.1	18
62	First-Principles Studies of the Activation of Oxygen Molecule and Its Role in Partial Oxidation of Methane on Boron-Doped Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2013, 117, 17485-17492.	3.1	17
63	Revealing the role of nitrogen dopants in tuning the electronic and optical properties of graphene quantum dots via a TD-DFT study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 28230-28237.	2.8	17
64	Rationale of the effects from dopants on C-H bond activation for sp ² hybridized nanostructured carbon catalysts. <i>Nanoscale</i> , 2015, 7, 16597-16600.	5.6	13
65	One-Step Synthesis of N/S Codoped Porous Carbon Cloth as a Sulfur Carrier for Lithium-Sulfur Batteries. <i>Energy Technology</i> , 2020, 8, 2000188.	3.8	11
66	Catalytic Property and Stability of Subnanometer Pt Cluster on Carbon Nanotube in Direct Propane Dehydrogenation. <i>Chinese Journal of Chemistry</i> , 2021, 39, 661-665.	4.9	11
67	Adsorption at Adsorption Sites: Halogen Atoms on Alkali Halide Surfaces. <i>Physical Review Letters</i> , 2006, 97, 046802.	7.8	10
68	The Unexpected Reactivity of the Carbon Sites on the Nanostructured Carbon Catalysts towards the C-H Bond Activation from the Analysis of the Aromaticity. <i>Chemistry - an Asian Journal</i> , 2016, 11, 1668-1671.	3.3	10
69	A Deoxygenation Method for Deprotection of Ketones and Aldehydes Using a Graphene-Oxide-Based Co-catalysts System. <i>Advanced Synthesis and Catalysis</i> , 2019, 361, 3137-3145.	4.3	10
70	Halogenation of graphene triggered by heteroatom doping. <i>RSC Advances</i> , 2019, 9, 37507-37511.	3.6	10
71	Resolving the Mechanism Complexity of Oxidative Dehydrogenation of Hydrocarbons on Nanocarbon by Microkinetic Modeling. <i>ACS Catalysis</i> , 2020, 10, 14006-14014.	11.2	9
72	Theoretical studies on dynamics and thermochemistry of the reactions CF ₃ CHCl ₂ +Cl ⁺ CF ₃ CCl ₂ +HCl and CF ₃ CHFCl+Cl ⁺ CF ₃ CFCl+HCl. <i>Journal of Chemical Physics</i> , 2004, 120, 6019-6027.	3.0	5

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73	Revealing nature of active site and reaction mechanism of supported chromium oxide catalyst in propane direct dehydrogenation. <i>Molecular Catalysis</i> , 2021, 505, 111520.	2.0	5
74	Revealing the intrinsic relation between heteroatom dopants and graphene quantum dots as a bi-functional ORR/OER catalyst. <i>Molecular Catalysis</i> , 2022, 518, 112109.	2.0	4
75	DFT study on the active site of the monometric molybdenum anchored on silica for the selective oxidation of ethane to acetaldehyde. <i>Molecular Catalysis</i> , 2018, 460, 83-86.	2.0	3
76	Revealing the role of HBr in propane dehydrogenation on CeO ₂ (111) <i>via</i> DFT-based microkinetic simulation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 9718-9726.	2.8	3
77	A critical evaluation of the catalytic role of CO ₂ in propane dehydrogenation catalyzed by chromium oxide from a DFT-based microkinetic simulation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 11030-11038.	2.8	3
78	Probing the reaction mechanism of acetylene hydrochlorination on metal-free doped boron nitride: Decisive role of carbon dopant. <i>Applied Surface Science</i> , 2021, 566, 150710.	6.1	1