## Dong Zhai

## List of Publications by Year in descending order

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		471509	395702
35	1,360	17	33
papers	citations	h-index	g-index
36	36	36	2016
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Single-atomic cobalt sites embedded in hierarchically ordered porous nitrogen-doped carbon as a superior bifunctional electrocatalyst. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 12692-12697.	7.1	325
2	Isolated Single-Atom Ni–N <sub>5</sub> Catalytic Site in Hollow Porous Carbon Capsules for Efficient Lithium–Sulfur Batteries. Nano Letters, 2021, 21, 9691-9698.	9.1	167
3	In situ embedding Co9S8 into nitrogen and sulfur codoped hollow porous carbon as a bifunctional electrocatalyst for oxygen reduction and hydrogen evolution reactions. Applied Catalysis B: Environmental, 2019, 254, 186-193.	20.2	135
4	van der Waals Heterojunction between a Bottom-Up Grown Doped Graphene Quantum Dot and Graphene for Photoelectrochemical Water Splitting. ACS Nano, 2020, 14, 1185-1195.	14.6	100
5	Enhanced carbon dioxide conversion at ambient conditions via a pore enrichment effect. Nature Communications, 2020, $11$ , $4481$ .	12.8	74
6	High-Loading Single-Atomic-Site Silver Catalysts with an Ag <sub>1</sub> –C <sub>2</sub> N <sub>1</sub> Structure Showing Superior Performance for Epoxidation of Styrene. ACS Catalysis, 2021, 11, 4946-4954.	11.2	62
7	Dissolution and Absorption: A Molecular Mechanism of Mesopore Formation in Alkaline Treatment of Zeolite. Chemistry of Materials, 2015, 27, 67-74.	6.7	52
8	Origin of Dirac Cones in SiC Silagraphene: A Combined Density Functional and Tight-Binding Study. Journal of Physical Chemistry Letters, 2015, 6, 1333-1339.	4.6	41
9	Periodic DFT study on mechanism of selective catalytic reduction of NO via NH3 and O2 over the V2O5 (001) surface: Competitive sites and pathways. Journal of Catalysis, 2013, 305, 67-75.	6.2	33
10	Chiral Hydroxytetraphenylene-Catalyzed Asymmetric Conjugate Addition of Boronic Acids to Enones. Organic Letters, 2019, 21, 5040-5045.	<b>4.</b> 6	33
11	Theoretical Investigation of Water Gas Shift Reaction Catalyzed by Iron Group Carbonyl Complexes M(CO) <sub>5</sub> (M = Fe, Ru, Os). Journal of Physical Chemistry A, 2012, 116, 2529-2535.	2.5	31
12	A first-principles evaluation of the stability, accessibility, and strength of $Br\tilde{A}_{s}$ nsted acid sites in zeolites. Journal of Catalysis, 2017, 352, 627-637.	6.2	29
13	Theoretical and Experimental Evidence for the Carbon–Oxygen Group Enhancement of NO Reduction. Environmental Science & Technology, 2017, 51, 14209-14216.	10.0	28
14	In Silico Design of Covalent Organic Framework-Based Electrocatalysts. Jacs Au, 2021, 1, 1497-1505.	7.9	28
15	Unblocked intramolecular charge transfer for enhanced CO2 photoreduction enabled by an imidazolium-based ionic conjugated microporous polymer. Applied Catalysis B: Environmental, 2022, 300, 120719.	20.2	25
16	Grand Canonical Monte Carlo simulations for energy gases on PIM-1 polymer and silicalite-1. Chemical Engineering Science, 2012, 68, 101-107.	3.8	23
17	Silver-Modified Ba <sub>1â€"<i>x</i></sub> Co <sub>0.7</sub> Fe <sub>0.2</sub> Nb <sub>0.1</sub> O <sub>3â^î</sub> Perovskite Performing as a Cathodic Catalyst of Intermediate-Temperature Solid Oxide Fuel Cells. ACS Applied Materials & Diverge Catalyst of Intermediate Catalyst o	8.0	19
18	Bifunctional poly(ionic liquid) catalyst with dual-active-center for CO2 conversion: Synergistic effect of triazine and imidazolium motifs. Journal of CO2 Utilization, 2021, 54, 101778.	6.8	17

#	Article	IF	CITATIONS
19	Salenâ€Based Conjugated Microporous Polymers for Efficient Oxygen Evolution Reaction. Chemistry - A European Journal, 2020, 26, 7720-7726.	3.3	16
20	Advantages of bimetallic nitric oxide reduction catalysts consisting of heavy metals rich in hazardous wastes. Journal of Cleaner Production, 2019, 237, 117834.	9.3	15
21	Organic Anions Facilitate in Situ Synthesis of Mesoporous LTA Zeolites. Chemistry of Materials, 2019, 31, 1528-1536.	6.7	15
22	A Porphyrinâ€Based Covalent Organic Framework for Metalâ€Free Photocatalytic Aerobic Oxidative Coupling of Amines. Chemistry - A European Journal, 2021, 27, 14390-14395.	3.3	15
23	Practical Enantioselective Synthesis of Chiroptical Polymers of Intrinsic Microporosity with Circular Polarized Luminescence. Macromolecules, 2021, 54, 11180-11186.	4.8	13
24	Reactive molecular dynamics study of thermal decomposition of nanocarbon energetic composite materials. Computational Materials Science, 2017, 131, 126-131.	3.0	11
25	Electroplating sludge-derived spinel catalysts for NO removal via NH3 selective catalysis reduction. Applied Surface Science, 2020, 528, 146969.	6.1	11
26	Single-atom catalysts modified by molecular groups for electrochemical nitrogen reduction. Nano Research, 2022, 15, 9663-9669.	10.4	11
27	Effect of temperature on the diffusion mechanism of xylene isomers in a FAU zeolite: a molecular dynamics study. Physical Chemistry Chemical Physics, 2012, 14, 7296.	2.8	8
28	Molecular dynamics study on core-shell structure stability of aluminum encapsulated by nano-carbon materials. Chemical Physics Letters, 2017, 669, 192-195.	2.6	8
29	Van der Waals Heterostructures Based on Porous Graphene for Photocatalytic Water Splitting. Journal of Physical Chemistry C, 2022, 126, 7849-7858.	3.1	7
30	Insight into the Contribution of Isolated Mesopore on Diffusion in Hierarchical Zeolites: The Effect of Temperature. Industrial & Engineering Chemistry Research, 2018, 57, 5453-5463.	3.7	4
31	A dramatic conformational effect of multifunctional zwitterions on zeolite crystallization. Chemical Communications, 2020, 56, 14693-14696.	4.1	1
32	In silico design of new nitrogen-rich melamine-based porous polyamides applied to CO2/N2 separation. Chemical Physics Letters, 2021, 771, 138509.	2.6	1
33	In silico design of metal-free hydrophosphate catalysts for hydrogenation of CO2 to formate. Physical Chemistry Chemical Physics, 2022, 24, 2901-2908.	2.8	1
34	Synergetic effect between Pd <sup>2+</sup> and Ir <sup>4+</sup> species promoting direct ethane dehydrogenation into ethylene over bimetallic PdIr/AC catalysts. Catalysis Science and Technology, 0, ,	4.1	1
35	The mechanism of sugar produced from simple glycolaldehyde derivative at ambient conditions. International Journal of Quantum Chemistry, 2022, 122, .	2.0	0