

Li-Ming Yang

List of Publications by Year in descending order

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59
papers

3,611
citations

147726

31
h-index

133188

59
g-index

60
all docs

60
docs citations

60
times ranked

3305
citing authors

#	ARTICLE	IF	CITATIONS
1	Unveiling the Underlying Mechanism of Transition Metal Atoms Anchored Square Tetracyanoquinodimethane Monolayers as Electrocatalysts for N ₂ Fixation. Energy and Environmental Materials, 2022, 5, 533-542.	7.3	25
2	Unveiling the underlying mechanism of nitrogen fixation by a new class of electrocatalysts two-dimensional TM@g-C ₄ N ₃ monosheets. Applied Surface Science, 2022, 576, 151839.	3.1	37
3	Efficient modulation of the catalytic performance of electrocatalytic nitrogen reduction with transition metals anchored on N/O-codoped graphene by coordination engineering. Journal of Materials Chemistry A, 2022, 10, 1481-1496.	5.2	43
4	Single-atom catalysts based on two-dimensional metalloporphyrin monolayers for ammonia synthesis under ambient conditions. Nano Research, 2022, 15, 4039-4047.	5.8	46
5	Prognostication of two-dimensional transition-metal atoms embedded rectangular tetrafluorotetracyanoquinodimethane single-atom catalysts for high-efficiency electrochemical nitrogen reduction. Journal of Colloid and Interface Science, 2022, 621, 24-32.	5.0	10
6	Dual transition metal atoms embedded in N-doped graphene for electrochemical nitrogen fixation under ambient conditions. Journal of Materials Chemistry A, 2022, 10, 13527-13543.	5.2	30
7	The Evolution of Geometric Structures, Electronic Properties, and Chemical Bonding of Small Phosphorus-Boron Clusters. Condensed Matter, 2022, 7, 36.	0.8	2
8	Transition Metals Embedded Two-Dimensional Square Tetrafluorotetracyanoquinodimethane Monolayers as a Class of Novel Electrocatalysts for Nitrogen Reduction Reaction. ACS Applied Materials & Interfaces, 2022, 14, 25317-25325.	4.0	11
9	A Supported Palladium on Gallium-based Liquid Metal Catalyst for Enhanced Oxygen Reduction Reaction. Chemical Research in Chinese Universities, 2022, 38, 1219-1225.	1.3	7
10	Atomistic Structures, Stabilities, Electronic Properties, and Chemical Bonding of Boron-Aluminum Mixed Clusters B ₃ AlO _n (+n) (n=2-6). Journal of Cluster Science, 2021, 32, 1261-1276.	1.7	4
11	Properties and Detailed Adsorption of CO ₂ by M ₂ (dobpdc) with <i>N,N</i> -Dimethylethylenediamine Functionalization. Inorganic Chemistry, 2021, 60, 2656-2662.	1.9	11
12	CO ₂ Adsorption Properties of a <i>N,N</i> -Diethylethylenediamine-Appended M ₂ (dobpdc) Series of Materials and Their Detailed Microprocess. Crystal Growth and Design, 2021, 21, 2474-2480.	1.4	9
13	Single Atomic Cerium Sites with a High Coordination Number for Efficient Oxygen Reduction in Proton-Exchange Membrane Fuel Cells. ACS Catalysis, 2021, 11, 3923-3929.	5.5	156
14	Electrocatalytic Reduction of N ₂ Using Metal-Doped Borophene. ACS Applied Materials & Interfaces, 2021, 13, 14091-14101.	4.0	70
15	Two-Dimensional Single-Atom Catalyst TM ₃ (HAB) ₂ Monolayers for Electrocatalytic Dinitrogen Reduction Using Hierarchical High-Throughput Screening. ACS Applied Materials & Interfaces, 2021, 13, 26109-26122.	4.0	56
16	Tailoring Unsymmetrical-Coordinated Atomic Site in Oxide-Supported Pt Catalysts for Enhanced Surface Activity and Stability. Small, 2021, 17, e2101008.	5.2	20
17	Electrocatalytic Mechanism of N ₂ Reduction Reaction by Single-Atom Catalyst Rectangular TM-TCNQ Monolayers. ACS Applied Materials & Interfaces, 2021, 13, 29641-29653.	4.0	42
18	Structural revolution of atomically dispersed Mn sites dictates oxygen reduction performance. Nano Research, 2021, 14, 4512-4519.	5.8	40

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19	Compressive Strain Modulation of Single Iron Sites on Helical Carbon Support Boosts Electrocatalytic Oxygen Reduction. <i>Angewandte Chemie</i> , 2021, 133, 22904-22910.	1.6	4
20	Compressive Strain Modulation of Single Iron Sites on Helical Carbon Support Boosts Electrocatalytic Oxygen Reduction. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 22722-22728.	7.2	113
21	Ammonia Synthesis Using Single-Atom Catalysts Based on Two-Dimensional Organometallic Metal Phthalocyanine Monolayers under Ambient Conditions. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 608-621.	4.0	82
22	Computational Prediction of the Low-Temperature Ferromagnetic Semiconducting 2D SiN Monolayer. <i>Physica Status Solidi (B): Basic Research</i> , 2020, 257, 1900619.	0.7	15
23	Disclosing the microscopic mechanism and adsorption properties of CO ₂ capture in <i>N</i> -isopropylethylenediamine appended M ₂ (dobpdc) series. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 24614-24623.	1.3	13
24	Bi-Based Metal-Organic Framework Derived Leafy Bismuth Nanosheets for Carbon Dioxide Electroreduction. <i>Advanced Energy Materials</i> , 2020, 10, 2001709.	10.2	210
25	Structural evolution in boron-based clusters B ₅ Al _n O _{4-n} (n=1-4): Al atoms transition from the periphery of the planar W-shaped B ₅ ring to the vertex of the bipyramid. <i>European Physical Journal D</i> , 2020, 74, 1.	0.6	4
26	Elucidation of the Underlying Mechanism of CO ₂ Capture by Ethylenediamine-Functionalized M ₂ (dobpdc) (M = Mg, Sc, Zn). <i>Inorganic Chemistry</i> , 2020, 59, 16665-16671.	1.9	13
27	Unveiling the Molecular Mechanism of CO ₂ Capture in <i>N</i> -Methylethylenediamine-Grafted M ₂ (dobpdc). <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 14616-14626.	3.2	24
28	Atomistic Level Mechanism of CO ₂ Adsorption in <i>N</i> -Ethylenediamine-Functionalized M ₂ (dobpdc) Metal-Organic Frameworks. <i>Crystal Growth and Design</i> , 2020, 20, 6337-6345.	1.4	12
29	The structures, electronic properties, and chemical bonding of binary alloy boron-aluminum clusters series B ₄ Al _n O _{5-n} (n=1-5). <i>Materials Today Communications</i> , 2020, 24, 100914.	0.9	4
30	Adsorption Properties and Microscopic Mechanism of CO ₂ Capture in 1,1-Dimethyl-1,2-ethylenediamine-Grafted Metal-Organic Frameworks. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 18533-18540.	4.0	36
31	Formation Mechanism of Ammonium Carbamate for CO ₂ Uptake in <i>N,N</i> -Dimethylethylenediamine Grafted M ₂ (dobpdc). <i>Langmuir</i> , 2020, 36, 14104-14112.	1.6	9
32	First-Principles Investigations of Single Metal Atoms (Sc, Ti, V, Cr, Mn, and Ni) Embedded in Hexagonal Boron Nitride Nanosheets for the Catalysis of CO Oxidation. <i>Condensed Matter</i> , 2019, 4, 65.	0.8	19
33	Two-Dimensional Organometallic TM ₃ C ₁₂ S ₁₂ Monolayers for Electrocatalytic Reduction of CO ₂ . <i>Energy and Environmental Materials</i> , 2019, 2, 193-200.	7.3	34
34	Efficient electrocatalytic reduction of carbon dioxide by metal-doped <i>I</i> ₂ -borophene monolayers. <i>RSC Advances</i> , 2019, 9, 27710-27719.	1.7	49
35	Two-Dimensional Anti-Van Hove Hoff/Le Bel Array AlB ₆ with High Stability, Unique Motif, Triple Dirac Cones, and Superconductivity. <i>Journal of the American Chemical Society</i> , 2019, 141, 3630-3640.	6.6	154
36	Electrochemical reduction of CO ₂ by single atom catalyst TM-TCNQ monolayers. <i>Journal of Materials Chemistry A</i> , 2019, 7, 3805-3814.	5.2	103

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37	Electrocatalytic reduction of CO ₂ by two-dimensional transition metal porphyrin sheets. <i>Journal of Materials Chemistry A</i> , 2019, 7, 11944-11952.	5.2	110
38	Efficient and Selective Electroreduction of CO ₂ by Single-Atom Catalyst Two-Dimensional TM-Pc Monolayers. <i>ACS Sustainable Chemistry and Engineering</i> , 2018, 6, 15494-15502.	3.2	124
39	Mn-graphene single-atom catalyst evaluated for CO oxidation by computational screening. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	42
40	The initial stages of melting of graphene between 4000 K and 6000 K. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 3756-3762.	1.3	72
41	Covalent Triazine Frameworks via a Low-Temperature Polycondensation Approach. <i>Angewandte Chemie</i> , 2017, 129, 14337-14341.	1.6	83
42	Covalent Triazine Frameworks via a Low-Temperature Polycondensation Approach. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 14149-14153.	7.2	441
43	Interior Melting of the C ₃ B ₁₆ and C ₂ B ₁₄ Clusters Between 1000 K and 2000 K. <i>Condensed Matter</i> , 2017, 2, 35.	0.8	1
44	Properties of the Free-Standing Two-Dimensional Copper Monolayer. <i>Journal of Nanomaterials</i> , 2016, 2016, 1-6.	1.5	13
45	Computational Study of Quasi-2D Liquid State in Free Standing Platinum, Silver, Gold, and Copper Monolayers. <i>Condensed Matter</i> , 2016, 1, 1.	0.8	21
46	Coexistence of Three Ferroic Orders in the Multiferroic Compound [(CH ₃) ₄ N][Mn(N ₃) ₃] with Perovskite-Like Structure. <i>Chemistry - A European Journal</i> , 2016, 22, 7863-7870.	1.7	54
47	Halogenated MOF-5 variants show new configuration, tunable band gaps and enhanced optical response in the visible and near infrared. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 32319-32330.	1.3	35
48	Tunable magnetism in metal adsorbed fluorinated nanoporous graphene. <i>Scientific Reports</i> , 2016, 6, 31841.	1.6	12
49	Adding a new dimension to the chemistry of phosphorus and arsenic. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17586-17591.	1.3	39
50	Four Decades of the Chemistry of Planar Hypercoordinate Compounds. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 9468-9501.	7.2	217
51	Two-Dimensional Cu ₂ Si Monolayer with Planar Hexacoordinate Copper and Silicon Bonding. <i>Journal of the American Chemical Society</i> , 2015, 137, 2757-2762.	6.6	335
52	The new dimension of silver. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 19695-19699.	1.3	52
53	Post-anti-van't Hoff-Le Bel motif in atomically thin germanium-copper alloy film. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 17545-17551.	1.3	81
54	Exceptional CO ₂ working capacity in a heterodiamine-grafted metal-organic framework. <i>Chemical Science</i> , 2015, 6, 3697-3705.	3.7	127

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55	Narrow bandgap covalent-organic frameworks with strong optical response in the visible and infrared. <i>Journal of Materials Chemistry C</i> , 2015, 3, 2244-2254.	2.7	18
56	Ten new predicted covalent organic frameworks with strong optical response in the visible and near infrared. <i>Journal of Chemical Physics</i> , 2015, 142, 244706.	1.2	11
57	Glitter in a 2D monolayer. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 26036-26042.	1.3	68
58	Revealing unusual chemical bonding in planar hyper-coordinate Ni ₂ Ge and quasi-planar Ni ₂ Si two-dimensional crystals. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 26043-26048.	1.3	95
59	Tuning electronic and optical properties of a new class of covalent organic frameworks. <i>Journal of Materials Chemistry C</i> , 2014, 2, 2404.	2.7	32