Hai-Tao Yu

List of Publications by Year
in descending order

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55 papers	932 citations	623734 14 h-index	477307 29 g-index
55 all docs	55 docs citations	55 times ranked	1398 citing authors

#	Article	IF	Citations
1	Synthesis of Large Surfaceâ€Area gâ€C₃N₄ Comodified with MnO_x and Auâ€TiO₂ as Efficient Visibleâ€Light Photocatalysts for Fuel Production. Advanced Energy Materials, 2018, 8, 1701580.	19.5	157
2	Enhanced Cocatalyst-Free Visible-Light Activities for Photocatalytic Fuel Production of g-C₃N₄ by Trapping Holes and Transferring Electrons. Journal of Physical Chemistry C, 2016, 120, 98-107.	3.1	135
3	Edge-exposed MoS2 nanospheres assembled with SnS2 nanosheet to boost NO2 gas sensing at room temperature. Journal of Hazardous Materials, 2020, 393, 122325.	12.4	86
4	Controllable synthesis of MoS₂@MoO₂ nanonetworks for enhanced NO₂ room temperature sensing in air. Nanoscale, 2019, 11, 8554-8564.	5.6	50
5	Li1.2Mn0.54Ni0.13Co0.13O2 hollow hierarchical microspheres with enhanced electrochemical performances as cathode material for lithium-ion battery application. Electrochimica Acta, 2017, 237, 217-226.	5.2	41
6	Urchin-like V₂O₃/C Hollow Nanosphere Hybrid for High-Capacity and Long-Cycle-Life Lithium Storage. ACS Sustainable Chemistry and Engineering, 2017, 5, 11238-11245.	6.7	39
7	Mg-doped Li1.2Mn0.54Ni0.13Co0.13O2 nano flakes with improved electrochemical performance for lithium-ion battery application. Journal of Alloys and Compounds, 2018, 739, 607-615.	5.5	34
8	First-Principles Investigation of Stability and Structural Properties of the BaTiO3(110) Polar Surface. Journal of Physical Chemistry C, 2007, 111, 6343-6349.	3.1	32
9	Hollow and hierarchical Na2Li2Ti6O14 microspheres with high electrochemical performance as anode material for lithium-ion battery. Science China Materials, 2017, 60, 427-437.	6.3	30
10	Engineering the Work Function of Buckled Boron Î±-Sheet by Lithium Adsorption: A First-Principles Investigation. ACS Applied Materials & Interfaces, 2014, 6, 19690-19701.	8.0	26
11	Tuning the band gaps and work functions via topology and carbon concentration: a first-principles investigation of Cx(BN)y compounds. Physical Chemistry Chemical Physics, 2012, 14, 4391.	2.8	24
12	Firstâ€principles calculations of the stability and electronic properties of the PbTiO₃ (110) polar surface. Journal of Computational Chemistry, 2009, 30, 1785-1798.	3.3	18
13	CoWO4 nanopaticles wrapped by RGO as high capacity anode material for lithium ion batteries. Rare Metals, 2017, 36, 411-417.	7.1	17
14	Hollow and hierarchical Li1.2Mn0.54Ni0.13Co0.13O2 micro-cubes as promising cathode materials for lithium ion battery. Journal of Alloys and Compounds, 2019, 807, 151686.	5.5	15
15	Thermodynamic stability and transport properties of tavorite LiFeSO₄F as a cathode material for lithium-ion batteries. Journal of Materials Chemistry A, 2015, 3, 19728-19737.	10.3	14
16	A first-principles investigation of the stabilities and electronic properties of SrZrO₃(1â€‰1â€‰0)(1â€‰Ã—â€‰1) polar terminations. Journal of Physics Condensed Matter, 2014, 26, 395002.	1.8	13
17	Novel Î±- and Î²-type boron sheets: Theoretical insight into their structures, thermodynamic stability, and work functions. Chemical Physics Letters, 2016, 648, 81-86.	2.6	12
18	Biocarbon-templated synthesis of porous Niâ€“Co-O nanocomposites for room-temperature NH3 sensors. New Journal of Chemistry, 2018, 42, 17606-17614.	2.8	11

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19	Surface modification of Li1.2Mn0.54Ni0.13Co0.13O2 via an ionic conductive LiV3O8 as a cathode material for Li-ion batteries. Ionics, 2019, 25, 4567-4576.	2.4	11
20	Intramolecular cyclization reaction mechanism and regioselectivities of unsubstituted and benzene-substituted 4-penteniminyl radicals: A DFT investigation. Computational and Theoretical Chemistry, 2013, 1005, 75-83.	2.5	10
21	Imparting Î±-Borophene with High Work Function by Fluorine Adsorption: A First-Principles Investigation. Langmuir, 2021, 37, 11027-11040.	3.5	10
22	Effect of cation doping on the electrochemical properties of Li2MoO3 as a promising cathode material for lithium-ion battery. Ionics, 2020, 26, 4413-4422.	2.4	9
23	Experimental and theoretical investigation of structures and relative reactivity of Pr@C74 and Pr@C74(C6H3Cl2). Diamond and Related Materials, 2016, 64, 110-118.	3.9	8
24	Structures, stabilities and work functions of alkali-metal-adsorbed boron Î± 1-sheets. Chemical Research in Chinese Universities, 2017, 33, 631-637.	2.6	8
25	Enhanced field-emission properties of buckled Î±-borophene by means of Li decoration: a first-principles investigation. Physical Chemistry Chemical Physics, 2018, 20, 15139-15148.	2.8	8
26	Highly Effective Work Function Reduction of Î±â€Borophene via Caesium Decoration: A Firstâ€Principles Investigation. Advanced Theory and Simulations, 2020, 3, 1900249.	2.8	8
27	Improving the structural stability and electrochemical performance of Na₂Li₂Ti₆O₁₄ nanoparticles via MgF₂ coating. RSC Advances, 2019, 9, 15763-15771.	3.6	7
28	Cascade cyclization of 1-(2-yl-3-phenylprop-2-enyl)-6-oxo-1,6-dihydropyridine-2-carbonitrile radical: Mechanistic insights from DFT study. Computational and Theoretical Chemistry, 2014, 1044, 1-9.	2.5	6
29	Molecular structures of Pr@C₇₂ and Pr@C₇₂(C₆H₃Cl₂): a combined experimentalâ€“theoretical investigation. RSC Advances, 2015, 5, 97568-97578.	3.6	6
30	Experimental and theoretical evaluation of structures of Pr₂@C₇₂ and its functionalized adduct with adamantylidene carbene. RSC Advances, 2016, 6, 115113-115119.	3.6	6
31	Theoretical Investigation of Regioselectivity and Stereoselectivity in AIBN/HSnBu₃-Mediated Radical Cyclization of N-(2-Iodo-4,6-dimethylphenyl)-N,2-dimethyl-(2E)-butenamide. Journal of Physical Chemistry B, 2016, 120, 12950-12958.	2.6	6
32	Li2MoO3 microspheres with excellent electrochemical performances as cathode material for lithium-ion battery. Ionics, 2020, 26, 4401-4411.	2.4	6
33	The Structures and Stability of HNOS Isomers. Chinese Journal of Chemistry, 2003, 21, 30-35.	4.9	5
34	Electronic properties of BaTiO3 (110) polar terminations. Chemical Research in Chinese Universities, 2014, 30, 794-799.	2.6	5
35	First-principles investigation of stability diagram and electronic properties of SrHfO3 (110) polar terminations. Materials Chemistry and Physics, 2016, 174, 195-203.	4.0	5
36	Effect of F Dopant on the Structural Stability, Redox Mechanism, and Electrochemical Performance of Li 2 MoO 3 Cathode Materials. Advanced Sustainable Systems, 2020, 4, 2000104.	5.3	5

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37	Effect of Li Adsorption on Work Function Modulation of Bilayer Î±-Borophene: A Theoretical Study. Acta Chimica Sinica, 2020, 78, 344.	1.4	5
38	Theoretical investigation of the structures, stabilities, and vibrational and rotational spectroscopic parameters of linear HOMgNC and HMgNCO molecules by density functional theory and coupled-cluster method. New Journal of Chemistry, 2022, 46, 7879-7891.	2.8	5
39	Structure and Stability of Interstellar Molecule C₃S. Chinese Journal of Chemistry, 2002, 20, 1487-1493.	4.9	4
40	Does the Neophyl-like Rearrangement Play a Decisive Role in Intramolecular Cyclization of Iminyl Radicals? A Combined Quantum Chemistry and Numerical Simulation Investigation of the Cyclization Mechanism and Product Distributions of Bicyclic 2-Allyl-2-methyl-2,3-dihydro-1H-inden-1-iminyl Radical and Several Iminyl Model Compounds. Journal of Organic Chemistry, 2019, 84, 2721-2731.	3.2	4
41	Effects of adatom species on the structure, stability, and work function of adatom-Î±-borophene nanocomposites. Physical Chemistry Chemical Physics, 2022, 24, 8923-8939.	2.8	4
42	Predicting Potential Stable Isomers on the Singlet Surface of the [H,P,C,S] System by the MP2 and QCISD(T) Methods. Theoretical Chemistry Accounts, 2006, 117, 49-56.	1.4	3
43	Theoretical study on the reaction mechanism of CN radical with ketene. Science in China Series B: Chemistry, 2008, 51, 101-110.	0.8	3
44	Construction of six-membered nitrogen-heterocycles via intramolecular cyclization of iminyl radical: A theoretical perspective. Computational and Theoretical Chemistry, 2013, 1025, 52-57.	2.5	3
45	Understanding the thermal stability and bonding characteristic of Li x Ni0.5Mn1.5O4 as cathode materials for lithium-ion battery from first principles. Ionics, 2017, 23, 559-565.	2.4	3
46	Effects of Ru doping on the structural stability and electrochemical properties of Li₂MoO₃ cathode materials for Li-ion batteries. Dalton Transactions, 2022, 51, 8786-8794.	3.3	3
47	Structures and Stability of HNS2 Isomers. Chinese Journal of Chemistry, 2010, 20, 760-765.	4.9	2
48	A Density Functional Theory Investigation of the Tandem Radical Cyclization of 1-[2-Yl-3-(2-Methoxyphenyl)-prop-2-enyl]-6-oxo-1,6-dihydropyridine-2-carbonitrile. Australian Journal of Chemistry, 2016, 69, 319.	0.9	2
49	A density functional theory investigation of the fragmentation mechanism of deprotonated asparagine. Computational and Theoretical Chemistry, 2018, 1141, 45-52.	2.5	2
50	DFT investigation of hydrogen atom-abstraction reactions of NHC-boranes by various carbon-centered radicals: barriers and correlation analyses. RSC Advances, 2020, 10, 34752-34763.	3.6	2
51	DFT Investigation of Hydrogen Atom Abstraction from NHC-Boranes by Methyl, Ethyl and Cyanomethyl Radicalsâ€”Composition and Correlation Analysis of Kinetic Barriers. Molecules, 2020, 25, 4509.	3.8	2
52	First-principles study on the electronic and bonding properties of PbTiO3 (110) polar terminations. Chemical Research in Chinese Universities, 2015, 31, 825-829.	2.6	1
53	A combined density functional theory and numerical simulation investigation of levels of chirality transfer and regioselectivity for the radical cyclizations of N-methyl-, N-ethyl- and N-isopropyl-substituted ortho-halo-N-acryloylanilides. New Journal of Chemistry, 2018, 42, 9783-9790.	2.8	1
54	Calculation and investigation of end-effect for a high-precision planar magnetic levitation. , 2010, , .		0

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55	Impact analysis of different axis layouts of detached breakwater on flow and sediment transport. Arabian Journal of Geosciences, 2021, 14, 1.	1.3	0