Hai-Tao Yu

List of Publications by Year
in descending order

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	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
2	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
3	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
4	Impact analysis of different axis layouts of detached breakwater on flow and sediment transport. Arabian Journal of Geosciences, 2021, 14, 1.	1.3	0
5	Imparting Î±-Borophene with High Work Function by Fluorine Adsorption: A First-Principles Investigation. Langmuir, 2021, 37, 11027-11040.	3.5	10
6	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
7	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
8	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
9	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
10	Li2MoO3 microspheres with excellent electrochemical performances as cathode material for lithium-ion battery. Ionics, 2020, 26, 4401-4411.	2.4	6
11	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
12	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
13	Effect of Li Adsorption on Work Function Modulation of Bilayer Î±-Borophene: A Theoretical Study. Acta Chimica Sinica, 2020, 78, 344.	1.4	5
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	Improving the structural stability and electrochemical performance of Na₂Li₂Ti₆O₁₄ nanoparticles via MgF₂ coating. RSC Advances, 2019, 9, 15763-15771.	3.6	7
16	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
17	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
18	Controllable synthesis of MoS₂@MoO₂ nanonetworks for enhanced NO₂ room temperature sensing in air. Nanoscale, 2019, 11, 8554-8564.	5.6	50

#	Article	IF	Citations
19	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
20	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
21	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
22	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
23	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
24	A density functional theory investigation of the fragmentation mechanism of deprotonated asparagine. Computational and Theoretical Chemistry, 2018, 1141, 45-52.	2.5	2
25	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
26	CoWO4 nanopaticles wrapped by RGO as high capacity anode material for lithium ion batteries. Rare Metals, 2017, 36, 411-417.	7.1	17
27	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
28	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
29	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
30	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
31	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
32	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
33	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
34	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
35	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
36	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

#	Article	IF	Citations
37	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
38	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
39	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
40	Molecular structures of Pr@C₇₂ and Pr@C₇₂(C₆H₃Cl₂): a combined experimentalâ€“theoretical investigation. RSC Advances, 2015, 5, 97568-97578.	3.6	6
41	Electronic properties of BaTiO3 (110) polar terminations. Chemical Research in Chinese Universities, 2014, 30, 794-799.	2.6	5
42	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
43	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
44	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
45	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
46	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
47	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
48	Structures and Stability of HNS2 Isomers. Chinese Journal of Chemistry, 2010, 20, 760-765.	4.9	2
49	Calculation and investigation of end-effect for a high-precision planar magnetic levitation. , 2010, , .		0
50	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
51	Theoretical study on the reaction mechanism of CN radical with ketene. Science in China Series B: Chemistry, 2008, 51, 101-110.	0.8	3
52	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
53	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
54	The Structures and Stability of HNOS Isomers. Chinese Journal of Chemistry, 2003, 21, 30-35.	4.9	5

#	Article	IF	Citations
55	Structure and Stability of Interstellar Molecule C₃S. Chinese Journal of Chemistry, 2002, 20, 1487-1493.	4.9	4