An-An Wu

List of Publications by Year
in descending order

41 papers	1,080 citations	516710 16 h-index	414414 32 g-index
42 all docs	42 docs citations	42 times ranked	1380 citing authors

#	Article	IF	Citations
1	Synergizing Surface Hydride Species and Ru Clusters on Sm₂O₃ for Efficient Ammonia Synthesis. ACS Catalysis, 2022, 12, 2178-2190.	11.2	23
2	Insights into the Mechanism of Metal-Catalyzed Transformation of Oxime Esters: Metal-Bound Radical Pathway vs Free Radical Pathway. Journal of Organic Chemistry, 2022, 87, 6014-6024.	3.2	5
3	Auto-classification of biomass through characterization of their pyrolysis behaviors using thermogravimetric analysis with support vector machine algorithm: case study for tobacco. Biotechnology for Biofuels, 2021, 14, 106.	6.2	8
4	Insights into the mechanism of fatty acid photodecarboxylase: A theoretical investigation. Chemical Physics Letters, 2021, 771, 138550.	2.6	2
5	Developing Ideal Metalorganic Hydrides for Hydrogen Storage: From Theoretical Prediction to Rational Fabrication. , 2021, 3, 1417-1425.		13
6	Barium chromium nitride-hydride for ammonia synthesis. Chem Catalysis, 2021, 1, 1042-1054.	6.1	19
7	Enabling Semihydrogenation of Alkynes to Alkenes by Using a Calcium Palladium Complex Hydride. Journal of the American Chemical Society, 2021, 143, 20891-20897.	13.7	20
8	Metallo-N-Heterocycles - A new family of hydrogen storage material. Energy Storage Materials, 2020, 26, 198-202.	18.0	22
9	Biosynthesis and Chemical Diversification of Verucopeptin Leads to Structural and Functional Versatility. Organic Letters, 2020, 22, 4366-4371.	4.6	6
10	Pharmacological Targeting of Vacuolar H+-ATPase via Subunit V1G Combats Multidrug-Resistant Cancer. Cell Chemical Biology, 2020, 27, 1359-1370.e8.	5.2	13
11	xOPBE: A Specialized Functional for Accurate Prediction of 13C Chemical Shifts. Journal of Physical Chemistry A, 2020, 124, 5824-5831.	2.5	7
12	Sodium anilinideâ€“cyclohexylamide pair: synthesis, characterization, and hydrogen storage properties. Chemical Communications, 2020, 56, 1944-1947.	4.1	7
13	Single-handed supramolecular double helix of homochiral bis(N-amidothiourea) supported by double crossed Câ˜IÂ·Â·Â·S halogen bonds. Nature Communications, 2019, 10, 3610.	12.8	55
14	Chemoselectivity in Gold(I)-Catalyzed Propargyl Ester Reactions: Insights From DFT Calculations. Frontiers in Chemistry, 2019, 7, 609.	3.6	3
15	Reversible Hydrogen Uptake/Release over a Sodium Phenoxideâ€“Cyclohexanolate Pair. Angewandte Chemie, 2019, 131, 3134-3139.	2.0	6
16	RÃ¼cktitelbild: Reversible Hydrogen Uptake/Release over a Sodium Phenoxideâ€“Cyclohexanolate Pair (Angew. Chem. 10/2019). Angewandte Chemie, 2019, 131, 3262-3262.	2.0	0
17	Reversible Hydrogen Uptake/Release over a Sodium Phenoxideâ€“Cyclohexanolate Pair. Angewandte Chemie - International Edition, 2019, 58, 3102-3107.	13.8	23
18	Metalâ€catalyzed alkyne oxidation/C ïŁ¿ H functionalization: Effects of oxidant, temperature, and metal catalyst on chemoselectivity. Journal of Computational Chemistry, 2019, 40, 1038-1044.	3.3	2

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19	Accurate prediction of nuclear magnetic resonance shielding constants: An extension of the focal-point analysis method for magnetic parameter calculations (FPA-M) with improved efficiency. Journal of Chemical Physics, 2018, 149, 184101.	3.0	3
20	The new chemical insight for understanding the mechanism of Henry reaction over Cu(II) catalyst. Chemical Physics Letters, 2017, 673, 7-10.	2.6	6
21	Atomically Dispersed Pt on the Surface of Ni Particles: Synthesis and Catalytic Function in Hydrogen Generation from Aqueous Ammoniaâ€“Borane. ACS Catalysis, 2017, 7, 6762-6769.	11.2	169
22	New 12,8-Eudesmanolides from Eutypella sp. 1â€“15. Journal of Antibiotics, 2017, 70, 1029-1032.	2.0	13
23	Accessing 2â€Arylbenzofurans by Cu^I₂(pip)₂â€Catalyzed Tandem Coupling/Cyclization Reaction: Mechanistic Studies and Application to the Synthesis of Stemofuran A and Moracin M. Asian Journal of Organic Chemistry, 2016, 5, 1345-1352.	2.7	12
24	Fluorescence of a triple-stranded helicate iron(<scp>iii</scp>) complex from a novel bis-Î²-diketone ligand: synthesis, structure and spectroscopic studies. CrystEngComm, 2016, 18, 6624-6631.	2.6	6
25	Lithium Imide Synergy with 3d Transitionâ€Metal Nitrides Leading to Unprecedented Catalytic Activities for Ammonia Decomposition. Angewandte Chemie - International Edition, 2015, 54, 2950-2954.	13.8	76
26	Aspertetranones Aâ€“D, Putative Meroterpenoids from the Marine Algal-Associated Fungus Aspergillus sp. ZL0-1b14. Journal of Natural Products, 2015, 78, 2405-2410.	3.0	25
27	Two new spirooxindole alkaloids from rhizosphere strain Streptomyces sp. xzqh-9. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 4995-4998.	2.2	26
28	Accurate prediction of nuclear magnetic resonance shielding constants: Towards the accuracy of CCSD(T) complete basis set limit. Journal of Chemical Physics, 2013, 138, 124113.	3.0	20
29	Metathesis of alkali-metal amidoborane and FeCl3 in THF. Journal of Materials Chemistry, 2012, 22, 7478.	6.7	11
30	Theoretical Studies on Dehydrogenation Reactions in Mg2(BH4)2(NH2)2 Compounds. Chinese Journal of Chemical Physics, 2012, 25, 676-680.	1.3	8
31	DCMB that combines divideâ€andâ€conquer and mixedâ€basis set methods for accurate geometry optimizations, total energies, and vibrational frequencies of large molecules. Journal of Computational Chemistry, 2012, 33, 1421-1432.	3.3	4
32	XO: An extended ONIOM method for accurate and efficient modeling of large systems. Journal of Computational Chemistry, 2012, 33, 2142-2160.	3.3	42
33	Highly Enantioselective Henry Reactions of Aromatic Aldehydes Catalyzed by an Amino Alcoholâ€“Copper(II) Complex. Chemistry - A European Journal, 2012, 18, 10515-10518.	3.3	40
34	Assessment of Some Density Functional Theory Methods and Force Field Models in Describing Various Interaction Modes of Benzene Dimer. Chinese Journal of Chemical Physics, 2011, 24, 635-639.	1.3	7
35	XO: An extended ONIOM method for accurate and efficient geometry optimization of large molecules. Chemical Physics Letters, 2010, 498, 203-208.	2.6	60
36	X-ray and DFT Study of Glaucocalyxin A Compound with Cytotoxic Activity. Chinese Journal of Chemical Physics, 2009, 22, 275-284.	1.3	8

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37	EPR and DFT Study of the Polycyclic Aromatic Radical Cations from Friedel-Crafts Alkylation Reactions. Chinese Journal of Chemical Physics, 2009, 22, 51-56.	1.3	5
38	Geometric Dependence of the B3LYP-Predicted Magnetic Shieldings and Chemical Shifts. Journal of Physical Chemistry A, 2007, 111, 9431-9437.	2.5	70
39	Systematic studies on the computation of nuclear magnetic resonance shielding constants and chemical shifts: The density functional models. Journal of Computational Chemistry, 2007, 28, 2431-2442.	3.3	68
40	OPBE: A promising density functional for the calculation of nuclear shielding constants. Chemical Physics Letters, 2006, 421, 383-388.	2.6	120
41	Efficient algorithm for the spin-free valence bond theory. I. New strategy and primary expressions. International Journal of Quantum Chemistry, 1998, 67, 287-297.	2.0	47