An-An Wu

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Atomically Dispersed Pt on the Surface of Ni Particles: Synthesis and Catalytic Function in Hydrogen Generation from Aqueous Ammonia–Borane. ACS Catalysis, 2017, 7, 6762-6769.	11.2	169
2	OPBE: A promising density functional for the calculation of nuclear shielding constants. Chemical Physics Letters, 2006, 421, 383-388.	2.6	120
3	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
4	Geometric Dependence of the B3LYP-Predicted Magnetic Shieldings and Chemical Shifts. Journal of Physical Chemistry A, 2007, 111, 9431-9437.	2.5	70
5	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
6	XO: An extended ONIOM method for accurate and efficient geometry optimization of large molecules. Chemical Physics Letters, 2010, 498, 203-208.	2.6	60
7	Single-handed supramolecular double helix of homochiral bis(N-amidothiourea) supported by double crossed Câ^'l···S halogen bonds. Nature Communications, 2019, 10, 3610.	12.8	55
8	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
9	XO: An extended ONIOM method for accurate and efficient modeling of large systems. Journal of Computational Chemistry, 2012, 33, 2142-2160.	3.3	42
10	Highly Enantioselective Henry Reactions of Aromatic Aldehydes Catalyzed by an Amino Alcohol–Copper(II) Complex. Chemistry - A European Journal, 2012, 18, 10515-10518.	3.3	40
11	Two new spirooxindole alkaloids from rhizosphere strain Streptomyces sp. xzqh-9. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 4995-4998.	2.2	26
12	Aspertetranones A–D, Putative Meroterpenoids from the Marine Algal-Associated Fungus <i>Aspergillus</i> sp. ZLO-1b14. Journal of Natural Products, 2015, 78, 2405-2410.	3.0	25
13	Reversible Hydrogen Uptake/Release over a Sodium Phenoxide–Cyclohexanolate Pair. Angewandte Chemie - International Edition, 2019, 58, 3102-3107.	13.8	23
14	Synergizing Surface Hydride Species and Ru Clusters on Sm ₂ O ₃ for Efficient Ammonia Synthesis. ACS Catalysis, 2022, 12, 2178-2190.	11.2	23
15	Metallo-N-Heterocycles - A new family of hydrogen storage material. Energy Storage Materials, 2020, 26, 198-202.	18.0	22
16	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
17	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
18	Barium chromium nitride-hydride for ammonia synthesis. Chem Catalysis, 2021, 1, 1042-1054.	6.1	19

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19	New 12,8-Eudesmanolides from Eutypella sp. 1–15. Journal of Antibiotics, 2017, 70, 1029-1032.	2.0	13
20	Pharmacological Targeting of Vacuolar H+-ATPase via Subunit V1G Combats Multidrug-Resistant Cancer. Cell Chemical Biology, 2020, 27, 1359-1370.e8.	5.2	13
21	Developing Ideal Metalorganic Hydrides for Hydrogen Storage: From Theoretical Prediction to Rational Fabrication. , 2021, 3, 1417-1425.		13
22	Accessing 2â€Arylbenzofurans by Cu ^I ₂ (pip) ₂ atalyzed 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
23	Metathesis of alkali-metal amidoborane and FeCl3 in THF. Journal of Materials Chemistry, 2012, 22, 7478.	6.7	11
24	X-ray and DFT Study of Glaucocalyxin A Compound with Cytotoxic Activity. Chinese Journal of Chemical Physics, 2009, 22, 275-284.	1.3	8
25	Theoretical Studies on Dehydrogenation Reactions in Mg2(BH4)2(NH2)2 Compounds. Chinese Journal of Chemical Physics, 2012, 25, 676-680.	1.3	8
26	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
27	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
28	xOPBE: A Specialized Functional for Accurate Prediction of 13C Chemical Shifts. Journal of Physical Chemistry A, 2020, 124, 5824-5831.	2.5	7
29	Sodium anilinide–cyclohexylamide pair: synthesis, characterization, and hydrogen storage properties. Chemical Communications, 2020, 56, 1944-1947.	4.1	7
30	Fluorescence of a triple-stranded helicate iron(<scp>iii</scp>) complex from a novel bis-β-diketone ligand: synthesis, structure and spectroscopic studies. CrystEngComm, 2016, 18, 6624-6631.	2.6	6
31	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
32	Reversible Hydrogen Uptake/Release over a Sodium Phenoxide–Cyclohexanolate Pair. Angewandte Chemie, 2019, 131, 3134-3139.	2.0	6
33	Biosynthesis and Chemical Diversification of Verucopeptin Leads to Structural and Functional Versatility. Organic Letters, 2020, 22, 4366-4371.	4.6	6
34	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
35	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
36	DCMB that combines divideâ€endâ€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

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37	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
38	Chemoselectivity in Gold(I)-Catalyzed Propargyl Ester Reactions: Insights From DFT Calculations. Frontiers in Chemistry, 2019, 7, 609.	3.6	3
39	Metalâ€catalyzed alkyne oxidation/C  H functionalization: Effects of oxidant, temperature, and metal catalyst on chemoselectivity. Journal of Computational Chemistry, 2019, 40, 1038-1044.	3.3	2
40	Insights into the mechanism of fatty acid photodecarboxylase: A theoretical investigation. Chemical Physics Letters, 2021, 771, 138550.	2.6	2
41	Rücktitelbild: Reversible Hydrogen Uptake/Release over a Sodium Phenoxide–Cyclohexanolate Pair (Angew. Chem. 10/2019). Angewandte Chemie, 2019, 131, 3262-3262.	2.0	0