Xue-Fang Yu

List of Publications by Year
in descending order

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23	1,107	840776 11	677142 22
papers	citations	h-index	g-index

23	23	23	1554
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The role of nitro group on the excited-state relaxation mechanism of P-Z base pair. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 267, 120549.	3.9	1
2	Triple proton transfer after water rearrangement in (2,6-aza)IndÂ·(H2O)2. Journal of Molecular Liquids, 2022, 353, 118847.	4.9	2
3	AIE mechanism of 2-(2-hydroxyphenyl) benzothiazole derivatives: CASPT2 and spin-flip study. Dyes and Pigments, 2022, 204, 110396.	3.7	2
4	A theoretical study on the excited-state deactivation paths for the Aâ€“5FU dimer. Physical Chemistry Chemical Physics, 2021, 23, 16089-16106.	2.8	3
5	Surface oxygen vacancies of Pd/Bi2MoO6-x acts as â€œElectron Bridgeâ€•to promote photocatalytic selective oxidation of alcohol. Applied Catalysis B: Environmental, 2021, 285, 119790.	20.2	90
6	Visible-near-infrared-responsive g-C3N4H+ reduced decatungstate with excellent performance for photocatalytic removal of petroleum hydrocarbon. Journal of Hazardous Materials, 2020, 381, 120994.	12.4	25
7	Screening NIR fluorescent sensor based on HBQ derivatives: A theoretical study. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 383, 111989.	3.9	6
8	Theoretical Design of Near-Infrared Fluorescent Sensor for F Anion Detection Based on 10-Hydroxybenzo[h]quinoline Backbone. ACS Omega, 2019, 4, 10516-10523.	3.5	6
9	Sensing mechanism of HBT based F anion fluorescence sensor: A theoretical study. Sensors and Actuators B: Chemical, 2019, 280, 162-170.	7.8	11
10	Photophysical properties and excited state proton transfer in 1,8-Dihydroxydibenzo[a,h]phenazine: A theoretical study. Journal of Photochemistry and Photobiology A: Chemistry, 2018, 353, 185-190.	3.9	5
11	Carbon Excess C₃N: A Potential Candidate as Li-Ion Battery Material. ACS Applied Materials & Interfaces, 2018, 10, 37135-37141.	8.0	44
12	Solvent effects on the excited-state double proton transfer mechanism in the 7-azaindole dimer: a TDDFT study with the polarizable continuum model. Physical Chemistry Chemical Physics, 2017, 19, 23289-23301.	2.8	15
13	Penta-graphene: A Promising Anode Material as the Li/Na-Ion Battery with Both Extremely High Theoretical Capacity and Fast Charge/Discharge Rate. ACS Applied Materials & Interfaces, 2016, 8, 35342-35352.	8.0	174
14	Atomic Insight into the Origin of Various Operation Voltages of Cation-Based Resistance Switches. ACS Applied Materials & Interfaces, 2016, 8, 31978-31985.	8.0	8
15	Monolayer Ti₂CO₂: A Promising Candidate for NH₃ Sensor or Capturer with High Sensitivity and Selectivity. ACS Applied Materials & Interfaces, 2015, 7, 13707-13713.	8.0	524
16	Structure and magnetic properties of open-ended silicon carbide nanotubes. RSC Advances, 2015, 5, 52754-52758.	3.6	2
17	The band gap modulation of monolayer Ti₂CO₂ by strain. RSC Advances, 2015, 5, 30438-30444.	3.6	82
18	Beryllium decorated armchair BC2N nanoribbons: coexistence of planar tetracoordinate carbon and nitrogen moieties. RSC Advances, 2015, 5, 73945-73950.	3.6	8

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19	Double-proton transfer mechanism in 1,8-dihydroxydibenzo[a,c]phenazine: a TDDFT and ab initio study. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	8
20	Protic vs Aprotic Solvent Effect on Proton Transfer in 3-Hydroxyisoquinoline: A Theoretical Study. Journal of Physical Chemistry A, 2015, 119, 11882-11890.	2.5	5
21	Theoretical Study on Water-Mediated Excited-State Multiple Proton Transfer in 7-Azaindole: Significance of Hydrogen Bond Rearrangement. Journal of Physical Chemistry A, 2012, 116, 10566-10573.	2.5	20
22	Theoretical study of the excitedâ€state double proton transfer in the (3â€methylâ€7â€azaindole)â€(7â€azaindole) heterodimer. Journal of Computational Chemistry, 2012, 33, 1701-1708.	3.3	17
23	Concerted or Stepwise Mechanism? CASPT2 and LC-TDDFT Study of the Excited-State Double Proton Transfer in the 7-Azaindole Dimer. Journal of Chemical Theory and Computation, 2011, 7, 1006-1015.	5.3	49