

Xue-Fang Yu

List of Publications by Year in descending order

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Version: 2024-02-01

23
papers

1,107
citations

840776

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677142

22
g-index

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all docs

23
docs citations

23
times ranked

1554
citing authors

#	ARTICLE	IF	CITATIONS
1	Monolayer Ti ₂ CO ₂ : A Promising Candidate for NH ₃ Sensor or Capturer with High Sensitivity and Selectivity. ACS Applied Materials & Interfaces, 2015, 7, 13707-13713.	8.0	524
2	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
3	Surface oxygen vacancies of Pd/Bi ₂ MoO _{6-x} acts as "Electron Bridge" to promote photocatalytic selective oxidation of alcohol. Applied Catalysis B: Environmental, 2021, 285, 119790.	20.2	90
4	The band gap modulation of monolayer Ti ₂ CO ₂ by strain. RSC Advances, 2015, 5, 30438-30444.	3.6	82
5	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
6	Carbon Excess C ₃ N: A Potential Candidate as Li-Ion Battery Material. ACS Applied Materials & Interfaces, 2018, 10, 37135-37141.	8.0	44
7	Visible-near-infrared-responsive g-C ₃ N ₄ H ₊ reduced decatungstate with excellent performance for photocatalytic removal of petroleum hydrocarbon. Journal of Hazardous Materials, 2020, 381, 120994.	12.4	25
8	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
9	Theoretical study of the excited-state double proton transfer in the (3-methyl-7-azaindole)-(7-azaindole) _{3,3} heterodimer. Journal of Computational Chemistry, 2012, 33, 1701-1708.		17
10	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
11	Sensing mechanism of HBT based F anion fluorescence sensor: A theoretical study. Sensors and Actuators B: Chemical, 2019, 280, 162-170.	7.8	11
12	Beryllium decorated armchair BC ₂ N nanoribbons: coexistence of planar tetracoordinate carbon and nitrogen moieties. RSC Advances, 2015, 5, 73945-73950.	3.6	8
13	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
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	Screening NIR fluorescent sensor based on HBQ derivatives: A theoretical study. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 383, 111989.	3.9	6
16	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
17	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
18	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

#	ARTICLE	IF	CITATIONS
19	A theoretical study on the excited-state deactivation paths for the A ⁺ 5FU dimer. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16089-16106.	2.8	3
20	Structure and magnetic properties of open-ended silicon carbide nanotubes. <i>RSC Advances</i> , 2015, 5, 52754-52758.	3.6	2
21	Triple proton transfer after water rearrangement in (2,6-aza)Ind ⁺ (H ₂ O) ₂ . <i>Journal of Molecular Liquids</i> , 2022, 353, 118847.	4.9	2
22	AIE mechanism of 2-(2-hydroxyphenyl) benzothiazole derivatives: CASPT2 and spin-flip study. <i>Dyes and Pigments</i> , 2022, 204, 110396.	3.7	2
23	The role of nitro group on the excited-state relaxation mechanism of P-Z base pair. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 267, 120549.	3.9	1