Weiwei Xie

List of Publications by Year in descending order

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21	461	687363 13	713466 21
papers	citations	h-index	g-index

21	21	21	437
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Revealing the key role of bonding states in surface chemisorption. Chemical Engineering Science, 2022, 249, 117345.	3.8	5
2	Understanding excited state properties of host materials in OLEDs: simulation of absorption spectrum of amorphous 4,4-bis(carbazol-9-yl)-2,2-biphenyl (CBP). Physical Chemistry Chemical Physics, 2022, , .	2.8	2
3	Efficient Surface Hopping Approach for Modeling Charge Transport in Organic Semiconductors. Journal of Chemical Theory and Computation, 2022, 18, 1264-1274.	5.3	4
4	Riemannian Surface on Carbon Anodes Enables Li-Ion Storage at â˜’35 Â°C. ACS Central Science, 2022, 8, 905-914.	11.3	5
5	Revealing the Role of d Orbitals of Transition-Metal-Doped Titanium Oxide on High-Efficient Oxygen Reduction. CCS Chemistry, 2021, 3, 180-188.	7.8	18
6	Interplay of structural dynamics and electronic effects in an engineered assembly of pentacene in a metalâ€“organic framework. Chemical Science, 2021, 12, 4477-4483.	7.4	18
7	Ab Initio Surface-Hopping Simulation of Femtosecond Transient-Absorption Pumpâ€“Probe Signals of Nonadiabatic Excited-State Dynamics Using the Doorwayâ€“Window Representation. Journal of Chemical Theory and Computation, 2021, 17, 2394-2408.	5.3	16
8	Modulating 3d Orbitals of Ni Atoms on Niâ€Pt Edge Sites Enables Highlyâ€Efficient Alkaline Hydrogen Evolution. Advanced Energy Materials, 2021, 11, 2101789.	19.5	30
9	Efficient Blue Light Emitting Diodes Based On Europium Halide Perovskites. Advanced Materials, 2021, 33, e2101903.	21.0	71
10	Exploration of Nontoxic Cs₃CeBr₆ for Violet Light-Emitting Diodes. ACS Energy Letters, 2021, 6, 4245-4254.	17.4	37
11	HAB79: A New Molecular Dataset for Benchmarking DFT and DFTB Electronic Couplings Against High-Level Ab-initio Calculations. Journal of Chemical Physics, 2021, 155, 234115.	3.0	14
12	Ab Initio Quasiclassical Simulation of Femtosecond Time-Resolved Two-Dimensional Electronic Spectra of Pyrazine. Journal of Physical Chemistry Letters, 2021, 12, 11736-11744.	4.6	9
13	Multi-faceted spectroscopic mapping of ultrafast nonadiabatic dynamics near conical intersections: A computational study. Journal of Chemical Physics, 2020, 153, 174111.	3.0	29
14	Photoinduced water oxidation in pyrimidineâ€“water clusters: a combined experimental and theoretical study. Physical Chemistry Chemical Physics, 2020, 22, 12502-12514.	2.8	16
15	Charge and Exciton Transfer Simulations Using Machine-Learned Hamiltonians. Journal of Chemical Theory and Computation, 2020, 16, 4061-4070.	5.3	30
16	Performance of Mixed Quantum-Classical Approaches on Modeling the Crossover from Hopping to Bandlike Charge Transport in Organic Semiconductors. Journal of Chemical Theory and Computation, 2020, 16, 2071-2084.	5.3	21
17	Photoinduced electron-driven proton transfer from water to an N-heterocyclic chromophore: nonadiabatic dynamics studies for pyridineâ€“water clusters. Physical Chemistry Chemical Physics, 2019, 21, 14073-14079.	2.8	28
18	Assessing the performance of trajectory surface hopping methods: Ultrafast internal conversion in pyrazine. Journal of Chemical Physics, 2019, 150, 154119.	3.0	44

#	Article	IF	Citations
19	Photoinduced hydrogen-transfer reactions in pyridine-water clusters: Insights from excited-state electronic-structure calculations. Chemical Physics, 2018, 515, 550-556.	1.9	10
20	Accuracy of trajectory surface-hopping methods: Test for a two-dimensional model of the photodissociation of phenol. Journal of Chemical Physics, 2017, 147, 184114.	3.0	43
21	State-specific tunneling lifetimes from classical trajectories: H-atom dissociation in electronically excited pyrrole. Journal of Chemical Physics, 2016, 144, 104105.	3.0	11