

Weiwei Xie

List of Publications by Year in descending order

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papers

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687363

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21
docs citations

21
times ranked

437
citing authors

#	ARTICLE	IF	CITATIONS
1	Efficient Blue Light Emitting Diodes Based On Europium Halide Perovskites. <i>Advanced Materials</i> , 2021, 33, e2101903.	21.0	71
2	Assessing the performance of trajectory surface hopping methods: Ultrafast internal conversion in pyrazine. <i>Journal of Chemical Physics</i> , 2019, 150, 154119.	3.0	44
3	Accuracy of trajectory surface-hopping methods: Test for a two-dimensional model of the photodissociation of phenol. <i>Journal of Chemical Physics</i> , 2017, 147, 184114.	3.0	43
4	Exploration of Nontoxic Cs ₃ CeBr ₆ for Violet Light-Emitting Diodes. <i>ACS Energy Letters</i> , 2021, 6, 4245-4254.	17.4	37
5	Charge and Exciton Transfer Simulations Using Machine-Learned Hamiltonians. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4061-4070.	5.3	30
6	Modulating 3d Orbitals of Ni Atoms on Ni ₄ Pt Edge Sites Enables Highly Efficient Alkaline Hydrogen Evolution. <i>Advanced Energy Materials</i> , 2021, 11, 2101789.	19.5	30
7	Multi-faceted spectroscopic mapping of ultrafast nonadiabatic dynamics near conical intersections: A computational study. <i>Journal of Chemical Physics</i> , 2020, 153, 174111.	3.0	29
8	Photoinduced electron-driven proton transfer from water to an N-heterocyclic chromophore: nonadiabatic dynamics studies for pyridine-water clusters. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 14073-14079.	2.8	28
9	Performance of Mixed Quantum-Classical Approaches on Modeling the Crossover from Hopping to Bandlike Charge Transport in Organic Semiconductors. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2071-2084.	5.3	21
10	Revealing the Role of d Orbitals of Transition-Metal-Doped Titanium Oxide on High-Efficient Oxygen Reduction. <i>CCS Chemistry</i> , 2021, 3, 180-188.	7.8	18
11	Interplay of structural dynamics and electronic effects in an engineered assembly of pentacene in a metal-organic framework. <i>Chemical Science</i> , 2021, 12, 4477-4483.	7.4	18
12	Photoinduced water oxidation in pyrimidine-water clusters: a combined experimental and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 12502-12514.	2.8	16
13	Ab Initio Surface-Hopping Simulation of Femtosecond Transient-Absorption Pump-Probe Signals of Nonadiabatic Excited-State Dynamics Using the Doorway Window Representation. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2394-2408.	5.3	16
14	HAB79: A New Molecular Dataset for Benchmarking DFT and DFTB Electronic Couplings Against High-Level Ab-initio Calculations. <i>Journal of Chemical Physics</i> , 2021, 155, 234115.	3.0	14
15	State-specific tunneling lifetimes from classical trajectories: H-atom dissociation in electronically excited pyrrole. <i>Journal of Chemical Physics</i> , 2016, 144, 104105.	3.0	11
16	Photoinduced hydrogen-transfer reactions in pyridine-water clusters: Insights from excited-state electronic-structure calculations. <i>Chemical Physics</i> , 2018, 515, 550-556.	1.9	10
17	Ab Initio Quasiclassical Simulation of Femtosecond Time-Resolved Two-Dimensional Electronic Spectra of Pyrazine. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 11736-11744.	4.6	9
18	Revealing the key role of bonding states in surface chemisorption. <i>Chemical Engineering Science</i> , 2022, 249, 117345.	3.8	5

#	ARTICLE	IF	CITATIONS
19	Riemannian Surface on Carbon Anodes Enables Li-Ion Storage at ~ 35 $^{\circ}\text{C}$. ACS Central Science, 2022, 8, 905-914.	11.3	5
20	Efficient Surface Hopping Approach for Modeling Charge Transport in Organic Semiconductors. Journal of Chemical Theory and Computation, 2022, 18, 1264-1274.	5.3	4
21	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