Weibin Chu

List of Publications by Year
in descending order

32	1,414	393982	433756
papers	citations	19 h-index	31 g-index

33	33	33	986
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Effects of oxygen vacancies on the photoexcited carrier lifetime in rutile TiO₂. Physical Chemistry Chemical Physics, 2022, 24, 4743-4750.	1.3	8
2	Interpolating Nonadiabatic Molecular Dynamics Hamiltonian with Inverse Fast Fourier Transform. Journal of Physical Chemistry Letters, 2022, 13, 331-338.	2.1	8
3	Dimensionality reduction in machine learning for nonadiabatic molecular dynamics: Effectiveness of elemental sublattices in lead halide perovskites. Journal of Chemical Physics, 2022, 156, 054110.	1.2	4
4	Control of Polaronic Behavior and Carrier Lifetimes via Metal and Anion Alloying in Chalcogenide Perovskites. Journal of Physical Chemistry Letters, 2022, 13, 4955-4962.	2.1	7
5	Electron-Volt Fluctuation of Defect Levels in Metal Halide Perovskites on a 100 ps Time Scale. Journal of Physical Chemistry Letters, 2022, 13, 5946-5952.	2.1	18
6	Ultrafast charge transfer coupled to quantum proton motion at molecule/metal oxide interface. Science Advances, 2022, 8, .	4.7	21
7	Two Dimensional MOene: From Superconductors to Direct Semiconductors and Weyl Fermions. Nano Letters, 2022, 22, 5592-5599.	4.5	8
8	Long-lived modulation of plasmonic absorption by ballistic thermal injection. Nature Nanotechnology, 2021, 16, 47-51.	15.6	40
9	Dynamics of Photoexcited Small Polarons in Transition-Metal Oxides. Journal of Physical Chemistry Letters, 2021, 12, 2191-2198.	2.1	41
10	Concentric Approximation for Fast and Accurate Numerical Evaluation of Nonadiabatic Coupling with Projector Augmented-Wave Pseudopotentials. Journal of Physical Chemistry Letters, 2021, 12, 3082-3089.	2.1	41
11	Why Hybrid Tin-Based Perovskites Simultaneously Improve the Structural Stability and Charge Carriersâ€™ Lifetime: Ab Initio Quantum Dynamics. ACS Applied Materials & Interfaces, 2021, 13, 16567-16575.	4.0	10
12	Strong Modulation of Band Gap, Carrier Mobility and Lifetime in Two-Dimensional Black Phosphorene through Acoustic Phonon Excitation. Journal of Physical Chemistry Letters, 2021, 12, 3960-3967.	2.1	30
13	Interpolating Nonadiabatic Molecular Dynamics Hamiltonian with Artificial Neural Networks. Journal of Physical Chemistry Letters, 2021, 12, 6070-6077.	2.1	29
14	Discovery of a Wurtzite-like Cu₂FeSnSe₄ Semiconductor Nanocrystal Polymorph and Implications for Related CuFeSe₂ Materials. ACS Nano, 2021, 15, 13463-13474.	7.3	10
15	Common Defects Accelerate Charge Carrier Recombination in CsSnI₃ without Creating Mid-Gap States. Journal of Physical Chemistry Letters, 2021, 12, 8699-8705.	2.1	31
16	Dependence between Structural and Electronic Properties of CsPbI₃: Unsupervised Machine Learning of Nonadiabatic Molecular Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 8672-8678.	2.1	26
17	Increasing Efficiency of Nonadiabatic Molecular Dynamics by Hamiltonian Interpolation with Kernel Ridge Regression. Journal of Physical Chemistry A, 2021, 125, 9191-9200.	1.1	8
18	Influence of intrinsic defects on the structure and dynamics of the mixed Pbâ€“Sn perovskite: first-principles DFT and NAMD simulations. Journal of Materials Chemistry A, 2021, 10, 234-244.	5.2	11

#	Article	IF	Citations
19	Significance of the Chemical Environment of an Element in Nonadiabatic Molecular Dynamics: Feature Selection and Dimensionality Reduction with Machine Learning. Journal of Physical Chemistry Letters, 2021, 12, 12026-12032.	2.1	11
20	Protecting hot carriers by tuning hybrid perovskite structures with alkali cations. Science Advances, 2020, 6, .	4.7	54
21	Accurate Computation of Nonadiabatic Coupling with Projector Augmented-Wave Pseudopotentials. Journal of Physical Chemistry Letters, 2020, 11, 10073-10080.	2.1	65
22	Long-Lived Hot Electron in a Metallic Particle for Plasmonics and Catalysis: Ab Initio Nonadiabatic Molecular Dynamics with Machine Learning. ACS Nano, 2020, 14, 10608-10615.	7.3	46
23	Structural Deformation Controls Charge Losses in MAPbI₃: Unsupervised Machine Learning of Nonadiabatic Molecular Dynamics. ACS Energy Letters, 2020, 5, 1930-1938.	8.8	55
24	Tuning the Carrier Lifetime in Black Phosphorene through Family Atom Doping. Journal of Physical Chemistry Letters, 2020, 11, 4662-4667.	2.1	48
25	Low-frequency lattice phonons in halide perovskites explain high defect tolerance toward electron-hole recombination. Science Advances, 2020, 6, eaaw7453.	4.7	182
26	Soft Lattice and Defect Covalency Rationalize Tolerance of Î²â€CsPbI₃ Perovskite Solar Cells to Native Defects. Angewandte Chemie - International Edition, 2020, 59, 6435-6441.	7.2	147
27	CO₂ Photoreduction on Metal Oxide Surface Is Driven by Transient Capture of Hot Electrons: Ab Initio Quantum Dynamics Simulation. Journal of the American Chemical Society, 2020, 142, 3214-3221.	6.6	63
28	Soft Lattice and Defect Covalency Rationalize Tolerance of Î²â€CsPbI₃ Perovskite Solar Cells to Native Defects. Angewandte Chemie, 2020, 132, 6497-6503.	1.6	8
29	Suppression of Electronâ€“Hole Recombination by Intrinsic Defects in 2D Monoelemental Material. Journal of Physical Chemistry Letters, 2019, 10, 6151-6158.	2.1	62
30	Ab initio nonadiabatic molecular dynamics investigations on the excited carriers in condensed matter systems. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1411.	6.2	194
31	Ultrafast Dynamics of Photongenerated Holes at a CH₃OH/TiO₂ Rutile Interface. Journal of the American Chemical Society, 2016, 138, 13740-13749.	6.6	126
32	High Photoreactivity on a Reconstructed Anatase TiO₂(001) Surface Predicted by Ab Initio Nonadiabatic Molecular Dynamics. Journal of Physical Chemistry Letters, 0, , 5766-5775.	2.1	2