

Hiroki Uratani

List of Publications by Year in descending order

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papers

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citations

1163117

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12
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12
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907
citing authors

#	ARTICLE	IF	CITATIONS
1	(Invited) Simulating Dynamic Excitons Via Quantum Molecular Dynamics: A Case Study in Lead Halide Perovskites. ECS Meeting Abstracts, 2022, MA2022-01, 904-904.	0.0	0
2	Trajectory Surface Hopping Approach to Condensed-Phase Nonradiative Relaxation Dynamics Using Divide-and-Conquer Spin-Flip Time-Dependent Density-Functional Tight Binding. Journal of Chemical Theory and Computation, 2021, 17, 1290-1300.	5.3	11
3	Scalable Ehrenfest Molecular Dynamics Exploiting the Locality of Density-Functional Tight-Binding Hamiltonian. Journal of Chemical Theory and Computation, 2021, 17, 7384-7396.	5.3	7
4	Quantum mechanical molecular dynamics simulations of polaron formation in methylammonium lead iodide perovskite. Physical Chemistry Chemical Physics, 2020, 22, 97-106.	2.8	23
5	Fast Nonadiabatic Molecular Dynamics via Spin-Flip Time-Dependent Density-Functional Tight-Binding Approach: Application to Nonradiative Relaxation of Tetraphenylethylene with Locked Aromatic Rings. Journal of Chemical Theory and Computation, 2020, 16, 7299-7313.	5.3	10
6	Non-adiabatic molecular dynamics with divide-and-conquer type large-scale excited-state calculations. Journal of Chemical Physics, 2020, 152, 224109.	3.0	14
7	Simulating the Coupled Structural–Electronic Dynamics of Photoexcited Lead Iodide Perovskites. Journal of Physical Chemistry Letters, 2020, 11, 4448-4455.	4.6	16
8	Quantum Mechanical Molecular Dynamics Simulations of Polaron Formation in a Perovskite Solar Cell Material. Journal of Computer Chemistry Japan, 2019, 18, 142-144.	0.1	2
9	Effects of Titania Coatings on Hydrodesulfurization Catalysts: Insights from First-principles Calculations. Journal of the Japan Petroleum Institute, 2018, 61, 288-293.	0.6	0
10	Charge Carrier Trapping at Surface Defects of Perovskite Solar Cell Absorbers: A First-Principles Study. Journal of Physical Chemistry Letters, 2017, 8, 742-746.	4.6	228
11	Inorganic Lattice Fluctuation Induces Charge Separation in Lead Iodide Perovskites: Theoretical Insights. Journal of Physical Chemistry C, 2017, 121, 26648-26654.	3.1	10
12	Detailed analysis of charge transport in amorphous organic thin layer by multiscale simulation without any adjustable parameters. Scientific Reports, 2016, 6, 39128.	3.3	29