Hiroki Uratani

List of Publications by Year
in descending order

12	350	1163117 8	1372567 10
papers	citations	h-index	g-index

12	12	12	907
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	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
3	Quantum mechanical molecular dynamics simulations of polaron formation in methylammonium lead iodide perovskite. Physical Chemistry Chemical Physics, 2020, 22, 97-106.	2.8	23
4	Simulating the Coupled Structuralâ€“Electronic Dynamics of Photoexcited Lead Iodide Perovskites. Journal of Physical Chemistry Letters, 2020, 11, 4448-4455.	4.6	16
5	Non-adiabatic molecular dynamics with divide-and-conquer type large-scale excited-state calculations. Journal of Chemical Physics, 2020, 152, 224109.	3.0	14
6	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
7	Inorganic Lattice Fluctuation Induces Charge Separation in Lead Iodide Perovskites: Theoretical Insights. Journal of Physical Chemistry C, 2017, 121, 26648-26654.	3.1	10
8	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
9	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
10	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
11	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
12	(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