Takatoshi Fujita

List of Publications by Year
in descending order

27 papers	590 citations	623734 14 h-index	610901 24 g-index
27 all docs	27 docs citations	27 times ranked	664 citing authors

#	Article	IF	Citations
1	FMO-Based Investigations of Excited-State Dynamics in Molecular Aggregates. , 2021, , 547-566.		2
2	First-Principles Investigations of Electronically Excited States in Organic Semiconductors. , 2021, , 155-193.		1
3	Fragment-Based Excited-State Calculations Using the GW Approximation and the Betheâ€“Salpeter Equation. Journal of Physical Chemistry A, 2021, 125, 10580-10592.	2.5	11
4	Revisiting the Charge-Transfer States at Pentacene/C60 Interfaces with the GW/Betheâ€“Salpeter Equation Approach. Materials, 2020, 13, 2728.	2.9	2
5	Numerical aspect of large-scale electronic state calculation for flexible device material. Japan Journal of Industrial and Applied Mathematics, 2019, 36, 685-698.	0.9	11
6	Charge-transfer excited states in the donor/acceptor interface from large-scale GW calculations. Journal of Chemical Physics, 2019, 151, 114109.	3.0	9
7	Development of the Fragment Molecular Orbital Method for Calculating Nonlocal Excitations in Large Molecular Systems. Journal of Physical Chemistry A, 2018, 122, 3886-3898.	2.5	28
8	Thousand-atom ab initio calculations of excited states at organic/organic interfaces: toward first-principles investigations of charge photogeneration. Physical Chemistry Chemical Physics, 2018, 20, 26443-26452.	2.8	7
9	Development of the fragment-based COHSEX method for large and complex molecular systems. Physical Review B, 2018, 98, .	3.2	11
10	Relating stacking structures and charge transport in crystal polymorphs of the pyrrole-based Ï€-conjugated molecule. Organic Electronics, 2017, 49, 53-63.	2.6	11
11	Emulation of complex open quantum systems using superconducting qubits. Quantum Information Processing, 2017, 16, 1.	2.2	23
12	Assessing the accuracy of integral equation theories for nano-sized hydrophobic solutes in water. Journal of Chemical Physics, 2017, 147, 014110.	3.0	12
13	Coherent Dynamics of Mixed Frenkel and Charge-Transfer Excitons in Dinaphtho[2,3-b:2â€²3â€²-f]thieno[3,2-b]-thiophene Thin Films: The Importance of Hole Delocalization. Journal of Physical Chemistry Letters, 2016, 7, 1374-1380.	4.6	24
14	Fast Delocalization Leads To Robust Long-Range Excitonic Transfer in a Large Quantum Chlorosome Model. Nano Letters, 2015, 15, 1722-1729.	9.1	29
15	Linear-algebraic bath transformation for simulating complex open quantum systems. New Journal of Physics, 2014, 16, 123008.	2.9	16
16	A stochastic reorganizational bath model for electronic energy transfer. Journal of Chemical Physics, 2014, 140, 244103.	3.0	4
17	Theoretical characterization of excitation energy transfer in chlorosome light-harvesting antennae from green sulfur bacteria. Photosynthesis Research, 2014, 120, 273-289.	2.9	41
18	Atomistic Study of Energy Funneling in the Light-Harvesting Complex of Green Sulfur Bacteria. Journal of the American Chemical Society, 2014, 136, 2048-2057.	13.7	78

#	Article	IF	Citations
19	Memory-Assisted Exciton Diffusion in the Chlorosome Light-Harvesting Antenna of Green Sulfur Bacteria. Journal of Physical Chemistry Letters, 2012, 3, 2357-2361.	4.6	63
20	Ab initio path integral Monte Carlo simulations for water trimer with electron correlation effects. Computational and Theoretical Chemistry, 2012, 997, 7-13.	2.5	10
21	Ab Initio Path Integral Molecular Dynamics and Monte Carlo Simulations for Water Trimer and Oligopeptide. ACS Symposium Series, 2012, , 187-199.	0.5	0
22	Fragment molecular orbital calculations under periodic boundary condition. Chemical Physics Letters, 2011, 506, 112-116.	2.6	41
23	Ab initioPath Integral Molecular Dynamics Based on Fragment Molecular Orbital Method. Journal of the Physical Society of Japan, 2009, 78, 104723.	1.6	22
24	Accuracy of fragmentation in ab initio calculations of hydrated sodium cation. Chemical Physics Letters, 2009, 478, 295-300.	2.6	41
25	Effects of salt addition on strength and dynamics of hydrophobic interactions. Chemical Physics Letters, 2007, 434, 42-48.	2.6	22
26	Fragment molecular orbital calculations on large scale systems containing heavy metal atom. Chemical Physics Letters, 2006, 427, 159-165.	2.6	53
27	Effects of molecular motion on charge transfer/transport through DNA duplexes with and without base pair mismatch. Molecular Simulation, 2006, 32, 759-764.	2.0	18