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	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
2	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
3	Fragment molecular orbital calculations on large scale systems containing heavy metal atom. Chemical Physics Letters, 2006, 427, 159-165.	2.6	53
4	Accuracy of fragmentation in ab initio calculations of hydrated sodium cation. Chemical Physics Letters, 2009, 478, 295-300.	2.6	41
5	Fragment molecular orbital calculations under periodic boundary condition. Chemical Physics Letters, 2011, 506, 112-116.	2.6	41
6	Theoretical characterization of excitation energy transfer in chlorosome light-harvesting antennae from green sulfur bacteria. Photosynthesis Research, 2014, 120, 273-289.	2.9	41
7	Fast Delocalization Leads To Robust Long-Range Excitonic Transfer in a Large Quantum Chlorosome Model. Nano Letters, 2015, 15, 1722-1729.	9.1	29
8	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
9	Coherent Dynamics of Mixed Frenkel and Charge-Transfer Excitons in Dinaphtho[2,3-‹i›b‹/i›:2â€²3â€²-‹i›f‹/i›]thieno[3,2-‹i›b‹/i›]-thiophene Thin Films: The Importance of Hole Delocalization. Journal of Physical Chemistry Letters, 2016, 7, 1374-1380.	4.6	24
10	Emulation of complex open quantum systems using superconducting qubits. Quantum Information Processing, 2017, 16, 1.	2.2	23
11	Effects of salt addition on strength and dynamics of hydrophobic interactions. Chemical Physics Letters, 2007, 434, 42-48.	2.6	22
12	‹i›Ab initio‹/i›Path Integral Molecular Dynamics Based on Fragment Molecular Orbital Method. Journal of the Physical Society of Japan, 2009, 78, 104723.	1.6	22
13	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
14	Linear-algebraic bath transformation for simulating complex open quantum systems. New Journal of Physics, 2014, 16, 123008.	2.9	16
15	Assessing the accuracy of integral equation theories for nano-sized hydrophobic solutes in water. Journal of Chemical Physics, 2017, 147, 014110.	3.0	12
16	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
17	Development of the fragment-based COHSEX method for large and complex molecular systems. Physical Review B, 2018, 98, .	3.2	11
18	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

#	Article	IF	Citations
19	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
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	Charge-transfer excited states in the donor/acceptor interface from large-scale GW calculations. Journal of Chemical Physics, 2019, 151, 114109.	3.0	9
22	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
23	A stochastic reorganizational bath model for electronic energy transfer. Journal of Chemical Physics, 2014, 140, 244103.	3.0	4
24	Revisiting the Charge-Transfer States at Pentacene/C60 Interfaces with the GW/Betheâ€“Salpeter Equation Approach. Materials, 2020, 13, 2728.	2.9	2
25	FMO-Based Investigations of Excited-State Dynamics in Molecular Aggregates. , 2021, , 547-566.		2
26	First-Principles Investigations of Electronically Excited States in Organic Semiconductors. , 2021, , 155-193.		1
27	Ab Initio Path Integral Molecular Dynamics and Monte Carlo Simulations for Water Trimer and Oligopeptide. ACS Symposium Series, 2012, , 187-199.	0.5	0