Hiroyuki Tamura

List of Publications by Year
in descending order

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67	2,707	186265	182427
papers	citations	28 h-index	51 g-index

69	69	69	3065
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Absorption wavelength along chromophore low-barrier hydrogen bonds. IScience, 2022, 25, 104247.	4.1	7
2	The origin of unidirectional charge separation in photosynthetic reaction centers: nonadiabatic quantum dynamics of exciton and charge in pigmentâ€“protein complexes. Chemical Science, 2021, 12, 8131-8140.	7.4	26
3	Nature of Asymmetric Electron Transfer in the Symmetric Pathways of Photosystem I. Journal of Physical Chemistry B, 2021, 125, 2879-2885.	2.6	16
4	Long-Range Electron Tunneling from the Primary to Secondary Quinones in Photosystem II Enhanced by Hydrogen Bonds with a Nonheme Fe Complex. Journal of Physical Chemistry B, 2021, 125, 13460-13466.	2.6	4
5	Acquirement of water-splitting ability and alteration of the charge-separation mechanism in photosynthetic reaction centers. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 16373-16382.	7.1	46
6	Lanthanide-doped inorganic nanoparticles turn molecular triplet excitons bright. Nature, 2020, 587, 594-599.	27.8	135
7	Triplet Exciton Transfers and Tripletâ€“Triplet Annihilation in Anthracene Derivatives via Direct versus Superexchange Pathways Governed by Molecular Packing. Journal of Physical Chemistry A, 2020, 124, 7943-7949.	2.5	7
8	Quenching of Singlet Oxygen by Carotenoids via Ultrafast Superexchange Dynamics. Journal of Physical Chemistry A, 2020, 124, 5081-5088.	2.5	26
9	Singlet exciton fission via an intermolecular charge transfer state in coevaporated pentacene-perfluoropentacene thin films. Journal of Chemical Physics, 2019, 151, 164706.	3.0	22
10	Long-Range Exciton Diffusion via Singlet Revival Mechanism. Journal of Physical Chemistry Letters, 2019, 10, 7623-7628.	4.6	6
11	Robust singlet fission in pentacene thin films with tuned charge transfer interactions. Nature Communications, 2018, 9, 954.	12.8	76
12	Impact of charge-transfer excitons in regioregular polythiophene on the charge separation at polythiophene-fullerene heterojunctions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2018, 51, 014003.	1.5	27
13	Quantum dynamical studies of ultrafast charge separation in nanostructured organic polymer materials: Effects of vibronic interactions and molecular packing. International Journal of Quantum Chemistry, 2018, 118, e25502.	2.0	30
14	Ultrafast carbon monoxide photolysis and heme spin-crossover in myoglobin via nonadiabatic quantum dynamics. Nature Communications, 2018, 9, 4502.	12.8	48
15	Comparative Study of Single and Dual Gain-Narrowed Emission in Thiophene/Furan/Phenylene Co-Oligomer Single Crystals. Journal of Physical Chemistry C, 2017, 121, 2364-2368.	3.1	12
16	Ï€-electron Sâ€‰=â€‰Â½ quantum spin-liquid state in an ionic polyaromatic hydrocarbon. Nature Chemistry, 2017, 9, 635-643.	13.6	46
17	Dynamics of the triplet-pair state reveals the likely coexistence of coherent and incoherent singlet fission in crystalline hexacene. Nature Chemistry, 2017, 9, 341-346.	13.6	155
18	The entangled triplet pair state in acene and heteroacene materials. Nature Communications, 2017, 8, 15953.	12.8	171

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19	Chapter 11 Ultrafast Energy and Charge Transfer in Functional Molecular Nanoscale Aggregates. , 2017, , 407-436.		1
20	Ultrafast excitonic and charge transfer dynamics in nanostructured organic polymer materials. , 2016, , .		0
21	Control of optical and electrical properties of nanosheets by the chemical structure of the turning point in a foldable polymer. Nanoscale, 2016, 8, 14673-14681.	5.6	18
22	Two different ground states in K-intercalated polyacenes. Physical Review B, 2016, 93, .	3.2	18
23	Diabatization for Time-Dependent Density Functional Theory: Exciton Transfers and Related Conical Intersections. Journal of Physical Chemistry A, 2016, 120, 9341-9347.	2.5	38
24	Molecular Packing Determines Charge Separation in a Liquid Crystalline Bisthiopheneâ€“Perylene Diimide Donorâ€“Acceptor Material. Journal of Physical Chemistry Letters, 2016, 7, 1327-1334.	4.6	28
25	First-Principles Quantum Dynamics of Singlet Fission: Coherent versus Thermally Activated Mechanisms Governed by Molecular<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Ï€</mml:mi></mml:math>Stacking. Physical Review Letters, 2015, 115, 107401.	7.8	137
26	Concurrent Effects of Delocalization and Internal Conversion Tune Charge Separation at Regioregular Polythiopheneâ€“Fullerene Heterojunctions. Journal of Physical Chemistry Letters, 2015, 6, 1702-1708.	4.6	72
27	Large-scale conductivity-tensor calculations for Hall effects in time-dependent wave-packet diffusion method. Physical Review B, 2014, 90, .	3.2	9
28	Non-Markovian reduced dynamics of ultrafast charge transfer at an oligothiopheneâ€“fullerene heterojunction. Chemical Physics, 2014, 442, 111-118.	1.9	17
29	Exciton diffusion length and charge mobility in donor and acceptor materials in organic photovoltaics: Tetrabenzoporphyrin and silylmethyl[60] fullerene. Chemical Physics Letters, 2014, 598, 81-85.	2.6	13
30	Theoretical Study on the Mechanism of Free Carrier Formation from Interfacial Electron-Hole Pair. Hyomen Kagaku, 2014, 35, 615-620.	0.0	0
31	Potential Barrier and Excess Energy for Electronâ€“Hole Separation from the Charge-Transfer Exciton at Donorâ€“Acceptor Heterojunctions of Organic Solar Cells. Journal of Physical Chemistry C, 2013, 117, 15020-15025.	3.1	51
32	Ultrafast Charge Separation in Organic Photovoltaics Enhanced by Charge Delocalization and Vibronically Hot Exciton Dissociation. Journal of the American Chemical Society, 2013, 135, 16364-16367.	13.7	292
33	Theoretical Analysis on the Optoelectronic Properties of Single Crystals of Thiophene-furan-phenylene Co-Oligomers: Efficient Photoluminescence due to Molecular Bending. Journal of Physical Chemistry C, 2013, 117, 8072-8078.	3.1	30
34	Single crystal biphenyl end-capped furan-incorporated oligomers: influence of unusual packing structure on carrier mobility and luminescence. Journal of Materials Chemistry C, 2013, 1, 4163.	5.5	73
35	Influence of strong electron-phonon coupling and dynamic lattice disorder on the Hall effect in organic crystals. Physical Review B, 2013, 87, .	3.2	5
36	Laser-assisted field evaporation from insulators triggered by photoinduced hole accumulation. Physical Review B, 2012, 86, .	3.2	27

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37	Roles of intramolecular and intermolecular electron-phonon coupling on the formation and transport of large polarons in organic semiconductors. Physical Review B, 2012, 86, .	3.2	27
38	Role of intermolecular charge delocalization on electron transport in fullerene aggregates. Physical Review B, 2012, 85, .	3.2	48
39	Quantum dynamics of ultrafast charge transfer at an oligothiophene-fullerene heterojunction. Journal of Chemical Physics, 2012, 137, 22A540.	3.0	85
40	Exciton Dissociation at Thiophene/Fullerene Interfaces: The Electronic Structures and Quantum Dynamics. Journal of Physical Chemistry C, 2011, 115, 10205-10210.	3.1	102
41	Mechanism of laser assisted field evaporation from insulating oxides. Ultramicroscopy, 2011, 111, 567-570.	1.9	45
42	Coherent transfer via environment-induced vibronic resonance. Journal of Chemical Physics, 2009, 130, 214705.	3.0	12
43	Ultrafast Electronic Processes At Semiconductor Polymer Heterojunctions: A Molecular-Level, Quantum-Dynamical Analysis. , 2009, , .		1
44	Ab Initio Study of Excitation Energy Transfer between Quantum Dots and Dye Molecules. Journal of Physical Chemistry C, 2009, 113, 7548-7552.	3.1	28
45	Ultrafast Photophysics of Organic Semiconductor Junctions. Springer Series in Chemical Physics, 2009, , 183-212.	0.2	8
46	Phonon-Driven Exciton Dissociation at Donorâ"Acceptor Polymer Heterojunctions:â€‰ Direct versus Bridge-Mediated Vibronic Coupling Pathways. Journal of Physical Chemistry B, 2008, 112, 495-506.	2.6	39
47	Phonon-Driven Ultrafast Exciton Dissociation at Donor-Acceptor Polymer Heterojunctions. Physical Review Letters, 2008, 100, 107402.	7.8	89
48	Exciton dissociation at donor-acceptor polymer heterojunctions: Quantum nonadiabatic dynamics and effective-mode analysis. Journal of Chemical Physics, 2007, 126, 021103.	3.0	63
49	Nonadiabatic quantum dynamics based on a hierarchical electron-phonon model: Exciton dissociation in semiconducting polymers. Journal of Chemical Physics, 2007, 127, 034706.	3.0	52
50	Quantum dynamics of ultrafast photoinduced processes in organic semiconductors: exciton dissociation at polymer heterojunctions. Proceedings in Applied Mathematics and Mechanics, 2007, 7, 1130601-1130602.	0.2	2
51	Laser control of reactions of photoswitching functional molecules. Journal of Chemical Physics, 2006, 125, 034307.	3.0	32
52	Ab initio nonadiabatic quantum dynamics of cyclohexadiene/hexatriene ultrafast photoisomerization. Journal of Chemical Physics, 2006, 124, 084313.	3.0	78
53	A theoretical study of cyclohexadiene/hexatriene photochemical interconversion: multireference configuration interaction potential energy surfaces and transition probabilities for the radiationless decays. Chemical Physics Letters, 2005, 401, 487-491.	2.6	52
54	Ab initio study of nucleation on the diamond (100) surface during chemical vapor deposition with methyl and H radicals. Chemical Physics Letters, 2005, 406, 197-201.	2.6	18

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55	Multiconfigurational self-consistent field study of the silicon carbide (001) surface. Journal of Chemical Physics, 2003, 119, 10318-10324.	3.0	15
56	Effect of S and O on the growth of chemical-vapor deposition diamond (100) surfaces. Journal of Chemical Physics, 2001, 115, 5284-5291.	3.0	9
57	Quantum Chemical Calculations of Sulfur Doping Reactions in Diamond CVD. Japanese Journal of Applied Physics, 2001, 40, 2830-2832.	1.5	26
58	Periodic density functional study on adsorption properties of organic molecules on clean Al (111) surface. Applied Surface Science, 2000, 158, 38-42.	6.1	12
59	Molecular Dynamics Simulations of Adhesional Forces via Hydrocarbon Films. Japanese Journal of Applied Physics, 2000, 39, 4425-4426.	1.5	0
60	Nonlinear Susceptibility of Second Harmonic Generation Corresponded to the Diamond (100) Surface Structures. Japanese Journal of Applied Physics, 2000, 39, 1845-1848.	1.5	2
61	Computational Chemistry Study on Initial Stages of Nitridation of Silicon Surfaces. Japanese Journal of Applied Physics, 2000, 39, 4443-4446.	1.5	2
62	Adsorption Properties of CH3OH on Al (111) and Fe (100) Surfaces: A Periodic First-Principles Investigation. Japanese Journal of Applied Physics, 2000, 39, 4275-4278.	1.5	4
63	Periodic density-functional study on oxidation of diamond (100) surfaces. Physical Review B, 2000, 61, 11025-11033.	3.2	55
64	First-principle study on reactions of diamond (100) surfaces with hydrogen and methyl radicals. Physical Review B, 2000, 62, 16995-17003.	3.2	37
65	Molecular Dynamics Simulation of Friction of Hydrocarbon Thin Films. Langmuir, 1999, 15, 7816-7821.	3.5	48
66	Simulation of Atomic Force Microscopy Images of Cleaved Mica Surfaces. Journal of Physical Chemistry B, 1997, 101, 4260-4264.	2.6	13
67	Molecular dynamics simulation of the friction between talc (001) surfaces. Applied Surface Science, 1997, 119, 335-340.	6.1	14