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	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
2	The entangled triplet pair state in acene and heteroacene materials. Nature Communications, 2017, 8, 15953.	12.8	171
3	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
4	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
5	Lanthanide-doped inorganic nanoparticles turn molecular triplet excitons bright. Nature, 2020, 587, 594-599.	27.8	135
6	Exciton Dissociation at Thiophene/Fullerene Interfaces: The Electronic Structures and Quantum Dynamics. Journal of Physical Chemistry C, 2011, 115, 10205-10210.	3.1	102
7	Phonon-Driven Ultrafast Exciton Dissociation at Donor-Acceptor Polymer Heterojunctions. Physical Review Letters, 2008, 100, 107402.	7.8	89
8	Quantum dynamics of ultrafast charge transfer at an oligothiophene-fullerene heterojunction. Journal of Chemical Physics, 2012, 137, 22A540.	3.0	85
9	Ab initio nonadiabatic quantum dynamics of cyclohexadiene/hexatriene ultrafast photoisomerization. Journal of Chemical Physics, 2006, 124, 084313.	3.0	78
10	Robust singlet fission in pentacene thin films with tuned charge transfer interactions. Nature Communications, 2018, 9, 954.	12.8	76
11	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
12	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
13	Exciton dissociation at donor-acceptor polymer heterojunctions: Quantum nonadiabatic dynamics and effective-mode analysis. Journal of Chemical Physics, 2007, 126, 021103.	3.0	63
14	Periodic density-functional study on oxidation of diamond (100) surfaces. Physical Review B, 2000, 61, 11025-11033.	3.2	55
15	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
16	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
17	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
18	Molecular Dynamics Simulation of Friction of Hydrocarbon Thin Films. Langmuir, 1999, 15, 7816-7821.	3.5	48

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19	Role of intermolecular charge delocalization on electron transport in fullerene aggregates. Physical Review B, 2012, 85, .	3.2	48
20	Ultrafast carbon monoxide photolysis and heme spin-crossover in myoglobin via nonadiabatic quantum dynamics. Nature Communications, 2018, 9, 4502.	12.8	48
21	Ï€-electron Sâ€‰=â€‰Â½ quantum spin-liquid state in an ionic polyaromatic hydrocarbon. Nature Chemistry, 2017, 9, 635-643.	13.6	46
22	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
23	Mechanism of laser assisted field evaporation from insulating oxides. Ultramicroscopy, 2011, 111, 567-570.	1.9	45
24	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
25	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
26	First-principle study on reactions of diamond (100) surfaces with hydrogen and methyl radicals. Physical Review B, 2000, 62, 16995-17003.	3.2	37
27	Laser control of reactions of photoswitching functional molecules. Journal of Chemical Physics, 2006, 125, 034307.	3.0	32
28	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
29	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
30	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
31	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
32	Laser-assisted field evaporation from insulators triggered by photoinduced hole accumulation. Physical Review B, 2012, 86, .	3.2	27
33	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
34	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
35	Quantum Chemical Calculations of Sulfur Doping Reactions in Diamond CVD. Japanese Journal of Applied Physics, 2001, 40, 2830-2832.	1.5	26
36	Quenching of Singlet Oxygen by Carotenoids via Ultrafast Superexchange Dynamics. Journal of Physical Chemistry A, 2020, 124, 5081-5088.	2.5	26

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37	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
38	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
39	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
40	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
41	Two different ground states in K-intercalated polyacenes. Physical Review B, 2016, 93, .	3.2	18
42	Non-Markovian reduced dynamics of ultrafast charge transfer at an oligothiopheneâ€“fullerene heterojunction. Chemical Physics, 2014, 442, 111-118.	1.9	17
43	Nature of Asymmetric Electron Transfer in the Symmetric Pathways of Photosystem I. Journal of Physical Chemistry B, 2021, 125, 2879-2885.	2.6	16
44	Multiconfigurational self-consistent field study of the silicon carbide (001) surface. Journal of Chemical Physics, 2003, 119, 10318-10324.	3.0	15
45	Molecular dynamics simulation of the friction between talc (001) surfaces. Applied Surface Science, 1997, 119, 335-340.	6.1	14
46	Simulation of Atomic Force Microscopy Images of Cleaved Mica Surfaces. Journal of Physical Chemistry B, 1997, 101, 4260-4264.	2.6	13
47	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
48	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
49	Coherent transfer via environment-induced vibronic resonance. Journal of Chemical Physics, 2009, 130, 214705.	3.0	12
50	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
51	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
52	Large-scale conductivity-tensor calculations for Hall effects in time-dependent wave-packet diffusion method. Physical Review B, 2014, 90, .	3.2	9
53	Ultrafast Photophysics of Organic Semiconductor Junctions. Springer Series in Chemical Physics, 2009, , 183-212.	0.2	8
54	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

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55	Absorption wavelength along chromophore low-barrier hydrogen bonds. IScience, 2022, 25, 104247.	4.1	7
56	Long-Range Exciton Diffusion via Singlet Revival Mechanism. Journal of Physical Chemistry Letters, 2019, 10, 7623-7628.	4.6	6
57	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
58	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
59	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
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	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
63	Ultrafast Electronic Processes At Semiconductor Polymer Heterojunctions: A Molecular-Level, Quantum-Dynamical Analysis. , 2009, , .		1
64	Chapter 11 Ultrafast Energy and Charge Transfer in Functional Molecular Nanoscale Aggregates. , 2017, , 407-436.		1
65	Molecular Dynamics Simulations of Adhesional Forces via Hydrocarbon Films. Japanese Journal of Applied Physics, 2000, 39, 4425-4426.	1.5	0
66	Theoretical Study on the Mechanism of Free Carrier Formation from Interfacial Electron-Hole Pair. Hyomen Kagaku, 2014, 35, 615-620.	0.0	0
67	Ultrafast excitonic and charge transfer dynamics in nanostructured organic polymer materials. , 2016, , .		0