Koichi Yamashita

List of Publications by Citations

108 papers	2,911 citations	26 h-index	52 g-index
113 ext. papers	3,256 ext. citations	4.3 avg, IF	5.7 L-index

#	Paper	IF	Citations
108	Small Photocarrier Effective Masses Featuring Ambipolar Transport in Methylammonium Lead Iodide Perovskite: A Density Functional Analysis. *Journal of Physical Chemistry Letters*, **2013**, 4, 4213-6	6.4	543
107	Black Phosphorus as a High-Capacity, High-Capability Negative Electrode for Sodium-Ion Batteries: Investigation of the Electrode/Electrolyte Interface. *Chemistry of Materials*, **2016**, 28, 1625-1635	9.6	199
106	Charge Carrier Trapping at Surface Defects of Perovskite Solar Cell Absorbers: A First-Principles Study. *Journal of Physical Chemistry Letters*, **2017**, 8, 742-746	6.4	181
105	The mechanism of slow hot-hole cooling in lead-iodide perovskite: first-principles calculation on carrier lifetime from electron-phonon interaction. *Nano Letters*, **2015**, 15, 3103-8	11.5	121
104	Organic□Inorganic Hybrid Lead Iodide Perovskite Featuring Zero Dipole Moment Guanidinium Cations: A Theoretical Analysis. *Journal of Physical Chemistry C*, **2015**, 119, 4694-4701	3.8	108
103	Organic□Inorganic halide perovskites: an ambipolar class of materials with enhanced photovoltaic performances. *Journal of Materials Chemistry A*, **2015**, 3, 8981-8991	13	89
102	Theoretical Study of the Surface Complex between TiO2 and TCNQ Showing Interfacial Charge-Transfer Transitions. *Journal of Physical Chemistry Letters*, **2011**, 2, 1167-70	6.4	81
101	The Effects of the Organic-Inorganic Interactions on the Thermal Transport Properties of CH3NH3PbI3. *Nano Letters*, **2016**, 16, 2749-53	11.5	80
100	Remarkable Dependence of the Final Charge Separation Efficiency on the Donor-Acceptor Interaction in Photoinduced Electron Transfer. *Angewandte Chemie - International Edition*, **2016**, 55, 629-33	16.4	79
99	Ab initio studies on the interstellar molecules C3H2 and C3H and the mechanism for the neutral□neutral reaction C(3P)+C2H2. *Journal of Chemical Physics*, **1996**, 104, 6613-6627	3.9	68
98	Penetration Barrier of Water through Graphynes□Pores: First-Principles Predictions and Force Field Optimization. *Journal of Physical Chemistry Letters*, **2014**, 5, 751-5	6.4	66
97	Alternative, Lead-free, Hybrid Organic□Inorganic Perovskites for Solar Applications: A DFT Analysis. *Chemistry Letters*, **2015**, 44, 826-828	1.7	60
96	Significance of hydrogen bonding and other noncovalent interactions in determining octahedral tilting in the CHNHPbI hybrid organic-inorganic halide perovskite solar cell semiconductor. *Scientific Reports*, **2019**, 9, 50	4.9	57
95	The proton conduction mechanism in a material consisting of packed acids. *Chemical Science*, **2014**, 5, 4878-4887	9.4	55
94	Theoretical study on the structure of Na+-doped helium clusters: Path integral Monte Carlo calculations. *Journal of Chemical Physics*, **2000**, 112, 10966-10975	3.9	51
93	Electron-electron and electron-phonon correlation effects on the finite-temperature electronic and optical properties of zinc-blende GaN. *Physical Review B*, **2014**, 89,	3.3	38
92	Nature of the Electronic and Optical Excitations of Ruddlesden-Popper Hybrid Organic-Inorganic Perovskites: The Role of the Many-Body Interactions. *Journal of Physical Chemistry Letters*, **2018**, 9, 5891-5896	6.4	38

91	Electronic Schr□dinger equation with nonclassical nuclei. *Physical Review A*, **2014**, 89,	2.6	37
90	Comparative Study of Sodium and Lithium Intercalation and Diffusion Mechanism in Black Phosphorus from First-principles Simulation. *Chemistry Letters*, **2014**, 43, 1940-1942	1.7	36
89	Zero-Dimensional Hybrid Organic-Inorganic Halide Perovskite Modeling: Insights from First Principles. *Journal of Physical Chemistry Letters*, **2016**, 7, 888-99	6.4	35
88	Atomic-Scale Analysis of the RuO2/Water Interface under Electrochemical Conditions. *Journal of Physical Chemistry C*, **2016**, 120, 8096-8103	3.8	35
87	The dissociation of HNO. I. Potential energy surfaces for the X 1A?, □□1A?, and □□3A? states. *Journal of Chemical Physics*, **1997**, 107, 6603-6615	3.9	34
86	A density functional tight binding study of acetic acid adsorption on crystalline and amorphous surfaces of titania. *Molecules*, **2015**, 20, 3371-88	4.8	33
85	A theoretical study on laser control of a molecular nonadiabatic process by ultrashort chirped laser pulses. *Journal of Chemical Physics*, **1998**, 109, 1801-1809	3.9	33
84	Theoretical study of the low-lying electronic states of XeO and XeS. *Journal of Chemical Physics*, **1998**, 108, 1514-1521	3.9	32
83	Theoretical and Experimental Studies on Reaction Mechanism for Aerobic Alcohol Oxidation by Supported Ruthenium Hydroxide Catalysts. *Journal of Physical Chemistry C*, **2010**, 114, 10873-10880	3.8	29
82	First-principles study of fast Na diffusion in Na3P. *Chemical Physics Letters*, **2014**, 612, 129-133	2.5	24
81	Carbonate-Promoted Catalytic Activity of Potassium Cations for Soot Combustion by Gaseous Oxygen. *ChemCatChem*, **2014**, 6, 479-484	5.2	24
80	Ab initio theory for current-induced molecular switching: Melamine on Cu(001). *Physical Review B*, **2013**, 87,	3.3	24
79	Theoretical study on quantum control of photodissociation and photodesorption dynamics by femtosecond chirped laser pulses. *Journal of Chemical Physics*, **1999**, 110, 7756-7769	3.9	24
78	Do surfaces of positive electrostatic potential on different halogen derivatives in molecules attract? like attracting like!. *Journal of Computational Chemistry*, **2018**, 39, 343-350	3.5	24
77	Hybrid organic-inorganic CH NH PbI perovskite building blocks: Revealing ultra-strong hydrogen bonding and mulliken inner complexes and their implications in materials design. *Journal of Computational Chemistry*, **2017**, 38, 2802-2818	3.5	23
76	DFT study of anatase-derived TiO2 nanosheets/graphene hybrid materials. *Physica Status Solidi (B): Basic Research*, **2014**, 251, 1471-1479	1.3	23
75	Revealing the Chemistry between Band Gap and Binding Energy for Lead-/Tin-Based Trihalide Perovskite Solar Cell Semiconductors. *ChemSusChem*, **2018**, 11, 449-463	8.3	22
74	Excitons at the (001) surface of anatase: Spatial behavior and optical signatures. *Physical Review B*, **2011**, 84,	3.3	21

73	Theoretical Studies on Proton Transfer among a High Density of Acid Groups: Surface of Zirconium Phosphate with Adsorbed Water Molecules. *Journal of Physical Chemistry C*, **2011**, 115, 5599-5606	3.8	21
72	Can Combined Electrostatic and Polarization Effects Alone Explain the F⋯F Negative-Negative Bonding in Simple Fluoro-Substituted Benzene Derivatives? A First-Principles Perspective. *Computation*, **2018**, 6, 51	2.2	21
71	Synthesis of Quinoidal Fused Oligosiloles by Rhodium-Catalyzed Stitching Reaction and Theoretical Investigation of Their Properties. *Journal of the American Chemical Society*, **2017**, 139, 3861-3867	16.4	20
70	STM and laser-driven atom switch: An open-system density-matrix study of H/Si(100). *Physical Review B*, **2003**, 67,	3.3	20
69	Two-dimensional optical excitations in the mixed-valence Cs2Au2I6 fully inorganic double perovskite. *Journal of Materials Chemistry C*, **2018**, 6, 10197-10201	7.1	20
68	Development of a Classical Interatomic Potential for MAPbBr3. *Journal of Physical Chemistry C*, **2017**, 121, 3724-3733	3.8	19
67	Redox Reaction Mechanisms with Non-triiodide Mediators in Dye-Sensitized Solar Cells by Redox Potential Calculations. *Journal of Physical Chemistry Letters*, **2012**, 3, 3581-4	6.4	18
66	Dynamic behavior of the IRC in chemical laser systems. *Theoretica Chimica Acta*, **1982**, 60, 523-533		18
65	Role of Quantum-Confinement in Anatase Nanosheets. *Journal of Physical Chemistry Letters*, **2017**, 8, 3867-3873	6.4	17
64	First-Principle Calculations of Solvated Electrons at Protic Solvent⋯TiO2 Interfaces with Oxygen Vacancies. *Journal of Physical Chemistry C*, **2009**, 113, 7236-7245	3.8	17
63	Revealing Factors Influencing the Fluorine-Centered Non-Covalent Interactions in Some Fluorine-Substituted Molecular Complexes: Insights from First-Principles Studies. *ChemPhysChem*, **2018**, 19, 1486-1499	3.2	16
62	Parameterized Bases for Calculating Vibrational Spectra Directly from ab Initio Data Using Rectangular Collocation. *Journal of Chemical Theory and Computation*, **2012**, 8, 2053-61	6.4	16
61	Effects of vibrational relaxation on the photodesorption of NO from Pt(111): A density matrix study. *Journal of Chemical Physics*, **2003**, 119, 9710-9718	3.9	16
60	Palladium-Catalyzed Intramolecular C-H Arylation versus 1,5-Palladium Migration: A Theoretical Investigation. *Chemistry - an Asian Journal*, **2018**, 13, 2566-2572	4.5	14
59	Charge Storage Mechanism of RuO2/Water Interfaces. *Journal of Physical Chemistry C*, **2017**, 121, 18975-18981	3.8	10
58	Electron trapping at the lattice Ti atoms adjacent to the Nb dopant in Nb-doped rutile TiO2. *Journal of Materials Science*, **2012**, 47, 7522-7529	4.3	9
57	Towards Accurate Spectroscopic Identification of Species at Catalytic Surfaces: Anharmonic Vibrations of Formate on AuPt. *Materials Research Society Symposia Proceedings*, **2012**, 1484, 1		9
56	Quantum chemical calculations on Al-CVD using DMEAA: surface reaction mechanism of AlH3 on Al(111). *Molecular Physics*, **2003**, 101, 267-276	1.7	9

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54	Phase evolution of electrochemically potassium intercalated graphite. *Journal of Materials Chemistry A*, **2021**, 9, 11187-11200	13	9
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52	Influence of the aggregate state on band structure and optical properties of C60 computed with different methods. *Journal of Chemical Physics*, **2018**, 148, 204301	3.9	9
51	-1 Isomers of tethered bismethano[70]fullerene as electron acceptors in organic photovoltaics.. *RSC Advances*, **2018**, 8, 18316-18326	3.7	9
50	First-Principles Study of the Band Diagrams and Schottky-Type Barrier Heights of Aqueous TaN Interfaces. *ACS Applied Materials & Interfaces*, **2017**, 9, 9559-9566	9.5	8
49	Inorganic Lattice Fluctuation Induces Charge Separation in Lead Iodide Perovskites: Theoretical Insights. *Journal of Physical Chemistry C*, **2017**, 121, 26648-26654	3.8	8
48	Nonspectral Methods for Solving the Schr□dinger Equation for Electronic and Vibrational Problems. *Journal of Physical Chemistry Letters*, **2011**, 2, 2193-2199	6.4	8
47	Model calculation of the electron-phonon coupling in Cs/Cu(111). *Physical Review B*, **2008**, 78,	3.3	8
46	Thermal effect on the morphology and performance of organic photovoltaics. *Physical Chemistry Chemical Physics*, **2016**, 18, 26456-26465	3.6	8
45	Li and Na Interaction with Ti2C-MXene: A First-Principles Calculation. *Journal of Computer Chemistry Japan*, **2019**, 18, 84-94	0.2	8
44	Energy Alignment of Frontier Orbitals and Suppression of Charge Recombinations in P3HT/SWNT. *Journal of Physical Chemistry C*, **2015**, 119, 26258-26265	3.8	7
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42	A theoretical study of molecular conduction. V. NEGF-based MP2 approach. *International Journal of Quantum Chemistry*, **2009**, 109, 1834-1840	2.1	7
41	Theoretical studies of the potential energy surface and wavepacket dynamics of the Li3 system. *Theoretical Chemistry Accounts*, **1999**, 102, 226-236	1.9	6
40	Revealing the Cooperative Chemistry of the Organic Cation in the Methylammonium Lead Triiodide Perovskite Semiconductor System. *ChemistrySelect*, **2018**, 3, 7269-7282	1.8	6
39	Defects in crystalline PVDF: a density functional theory-density functional tight binding study. *Physical Chemistry Chemical Physics*, **2017**, 19, 7560-7567	3.6	5
38	Chalcogen Bonding in the Molecular Dimers of WCh (Ch = S, Se, Te): On the Basic Understanding of the Local Interfacial and Interlayer Bonding Environment in 2D Layered Tungsten Dichalcogenides.. *International Journal of Molecular Sciences*, **2022**, 23,	6.3	5

37	Dipole analyses for short-circuit current in organic photovoltaic devices of diketopyrrolopyrrole-based donor and PCBM. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	5
36	Electron wavepacket approaches to non-adiabatic transition processes in the internal rotational motion of H2CNH2+ Charge oscillation due to electronic coherence. *Chemical Physics Letters*, **2015**, 635, 345-349	2.5	4
35	Effect of Isotopic Substitution on Elementary Processes in Dye-Sensitized Solar Cells: Deuterated Amino-Phenyl Acid Dyes on TiO2. *Computation*, **2013**, 1, 1-15	2.2	4
34	Theoretical study of molecular conduction: I. Effective Green's function based on perturbation theory. *International Journal of Quantum Chemistry*, **2006**, 106, 803-813	2.1	4
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30	Theoretical Verification of Photoelectrochemical Water Oxidation Using Nanocrystalline TiO2 Electrodes. *Molecules*, **2015**, 20, 9732-44	4.8	3
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28	The Phosphorus Bond, or the Phosphorus-Centered Pnictogen Bond: The Covalently Bound Phosphorus Atom in Molecular Entities and Crystals as a Pnictogen Bond Donor.. *Molecules*, **2022**, 27,	4.8	3
27	The Nitrogen Bond, or the Nitrogen-Centered Pnictogen Bond: The Covalently Bound Nitrogen Atom in Molecular Entities and Crystals as a Pnictogen Bond Donor. *Compounds*, **2022**, 2, 80-110		3
26	A new implementation of ab initio ehrenfest dynamics using electronic configuration basis: Exact formulation with molecular orbital connection and effective propagation scheme with locally quasi-diabatic representation. *International Journal of Quantum Chemistry*, **2016**, 116, 1205-1213	2.1	2
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24	Laser-induced fluorescence of the CHFCHO radical and reaction of OH radicals with halogenated ethylenes. *Journal of Chemical Physics*, **2019**, 150, 174302	3.9	1
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22	Halogen in materials design: Fluoroammonium lead triiodide (FNH3PbI3) perovskite as a newly discovered dynamical bandgap semiconductor in 3D. *International Journal of Quantum Chemistry*, **2018**, 118, e25621	2.1	1
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16	A theoretical study on quantum control of photodissociation dynamics by ultrashort chirped laser pulses. *International Journal of Quantum Chemistry*, **1999**, 72, 525-532	2.1	1
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13	A Theoretical study on the charge and discharge states of Na-ion battery cathode material, Na FePO F. *Journal of Computational Chemistry*, **2019**, 40, 237-246	3.5	1
12	Theoretical investigation of [Ru(tpy)2]2+, [Ru(tpy)(bpy)(H2O)]2+ and [Ru(tpy)(bpy)(Cl)]+ complexes in acetone revisited: Inclusion of strong spin orbit couplings to quantum chemistry calculations. *Journal of Theoretical and Computational Chemistry*, **2016**, 15, 1650001	1.8	0
11	Importance of Side-Chains on Molecular Characteristics of Interacting Organic Molecules. *ACS Omega*, **2019**, 4, 10396-10404	3.9	
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9	Theoretical studies on a new pattern of laser-driven systems: towards elucidation of direct photo-injection in dye-sensitized solar cells. *Theoretical Chemistry Accounts*, **2011**, 130, 227-236	1.9	
8	The intrinsic reaction coordinate approach in polyatomic reaction dynamics. *International Journal of Quantum Chemistry*, **2009**, 24, 177-189	2.1	
7	Modeling and Simulation of Photocatalytic Reactions at TiO2 Surfaces37-75		
6	Control of Chemical Reactions by Using Chirped Laser Pulses. *ACS Symposium Series*, **2002**, 81-97	0.4	
5	A FLUX-FLUX CROSS-CORRELATION FUNCTION APPROACH TO SELF-DIFFUSION OF HYDROGEN ATOM ON A CU(111) SURFACE. *Journal of Theoretical and Computational Chemistry*, **2005**, 04, 209-223	1.8	
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2	Electronic and Optical Properties of Nitrogen-Doped Layered Manganese Oxides. *Ceramic Transactions*,135-140	0.1	

1 Laser-induced fluorescence of the trans-CHBrCHO radical. *Journal of Chemical Physics*, **2020**, 153, 104301. 3.9