Koichi Yamashita

List of Publications by Year
in descending order

113 papers	3,623 citations	172207 29 h-index	138251 58 g-index
113 all docs	113 docs citations	113 times ranked	6089 citing authors

#	Article	IF	Citations
1	Small Photocarrier Effective Masses Featuring Ambipolar Transport in Methylammonium Lead Iodide Perovskite: A Density Functional Analysis. Journal of Physical Chemistry Letters, 2013, 4, 4213-4216.	2.1	675
2	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.	3.2	238
3	Charge Carrier Trapping at Surface Defects of Perovskite Solar Cell Absorbers: A First-Principles Study. Journal of Physical Chemistry Letters, 2017, 8, 742-746.	2.1	228
4	The Mechanism of Slow Hot-Hole Cooling in Lead-Iodide Perovskite: First-Principles Calculation on Carrier Lifetime from Electronâ€“Phonon Interaction. Nano Letters, 2015, 15, 3103-3108.	4.5	140
5	Organicâ€“Inorganic Hybrid Lead Iodide Perovskite Featuring Zero Dipole Moment Guanidinium Cations: A Theoretical Analysis. Journal of Physical Chemistry C, 2015, 119, 4694-4701.	1.5	132
6	Organicâ€“inorganic halide perovskites: an ambipolar class of materials with enhanced photovoltaic performances. Journal of Materials Chemistry A, 2015, 3, 8981-8991.	5.2	109
7	The Effects of the Organicâ€“Inorganic Interactions on the Thermal Transport Properties of CH₃NH₃PbI₃. Nano Letters, 2016, 16, 2749-2753.	4.5	95
8	Significance of hydrogen bonding and other noncovalent interactions in determining octahedral tilting in the CH3NH3PbI3 hybrid organic-inorganic halide perovskite solar cell semiconductor. Scientific Reports, 2019, 9, 50.	1.6	95
9	Remarkable Dependence of the Final Charge Separation Efficiency on the Donorâ€“Acceptor Interaction in Photoinduced Electron Transfer. Angewandte Chemie - International Edition, 2016, 55, 629-633.	7.2	94
10	Theoretical Study of the Surface Complex between TiO₂ and TCNQ Showing Interfacial Charge-Transfer Transitions. Journal of Physical Chemistry Letters, 2011, 2, 1167-1170.	2.1	89
11	Penetration Barrier of Water through Graphynesâ€™ Pores: First-Principles Predictions and Force Field Optimization. Journal of Physical Chemistry Letters, 2014, 5, 751-755.	2.1	84
12	Ab initio studies on the interstellar molecules C3H2 and C3H and the mechanism for the neutralâ€“neutral reaction C(3P)+C2H2. Journal of Chemical Physics, 1996, 104, 6613-6627.	1.2	72
13	The proton conduction mechanism in a material consisting of packed acids. Chemical Science, 2014, 5, 4878-4887.	3.7	72
14	Alternative, Lead-free, Hybrid Organicâ€“Inorganic Perovskites for Solar Applications: A DFT Analysis. Chemistry Letters, 2015, 44, 826-828.	0.7	65
15	Theoretical study on the structure of Na+-doped helium clusters: Path integral Monte Carlo calculations. Journal of Chemical Physics, 2000, 112, 10966-10975.	1.2	55
16	Nature of the Electronic and Optical Excitations of Ruddlesdenâ€“Popper Hybrid Organicâ€“Inorganic Perovskites: The Role of the Many-Body Interactions. Journal of Physical Chemistry Letters, 2018, 9, 5891-5896.	2.1	51
17	Electron-electron and electron-phonon correlation effects on the finite-temperature electronic and optical properties of zinc-blende GaN. Physical Review B, 2014, 89, .	1.1	49
18	Atomic-Scale Analysis of the RuO₂/Water Interface under Electrochemical Conditions. Journal of Physical Chemistry C, 2016, 120, 8096-8103.	1.5	41

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19	The dissociation of HNO. I. Potential energy surfaces for the XÌƒâ€‰1Aâ€², Ãƒâ€‰1Aâ€³, and Ã£â€‰3Aâ€³ states. Journal of Chemical Physics, 1997, 107, 6603-6615.	1.2	40
20	Electronic SchrÃ¶dinger equation with nonclassical nuclei. Physical Review A, 2014, 89, .	1.0	40
21	Comparative Study of Sodium and Lithium Intercalation and Diffusion Mechanism in Black Phosphorus from First-principles Simulation. Chemistry Letters, 2014, 43, 1940-1942.	0.7	40
22	A Density Functional Tight Binding Study of Acetic Acid Adsorption on Crystalline and Amorphous Surfaces of Titania. Molecules, 2015, 20, 3371-3388.	1.7	40
23	Zero-Dimensional Hybrid Organicâ€“Inorganic Halide Perovskite Modeling: Insights from First Principles. Journal of Physical Chemistry Letters, 2016, 7, 888-899.	2.1	40
24	A theoretical study on laser control of a molecular nonadiabatic process by ultrashort chirped laser pulses. Journal of Chemical Physics, 1998, 109, 1801-1809.	1.2	37
25	Theoretical study of the low-lying electronic states of XeO and XeS. Journal of Chemical Physics, 1998, 108, 1514-1521.	1.2	33
26	Do surfaces of positive electrostatic potential on different halogen derivatives in molecules attract? like attracting like!. Journal of Computational Chemistry, 2018, 39, 343-350.	1.5	33
27	Hybrid organicâ€“inorganic CH₃NH₃PbI₃ perovskite building blocks: Revealing ultraâ€strong hydrogen bonding and mulliken inner complexes and their implications in materials design. Journal of Computational Chemistry, 2017, 38, 2802-2818.	1.5	32
28	Can Combined Electrostatic and Polarization Effects Alone Explain the FÂ·Â·Â·F Negative-Negative Bonding in Simple Fluoro-Substituted Benzene Derivatives? A First-Principles Perspective. Computation, 2018, 6, 51.	1.0	32
29	Two-dimensional optical excitations in the mixed-valence Cs₂Au₂I₆ fully inorganic double perovskite. Journal of Materials Chemistry C, 2018, 6, 10197-10201.	2.7	32
30	Development of a Classical Interatomic Potential for MAPbBr₃. Journal of Physical Chemistry C, 2017, 121, 3724-3733.	1.5	31
31	Unveiling charge dynamics of visible light absorbing oxysulfide for efficient overall water splitting. Nature Communications, 2021, 12, 7055.	5.8	31
32	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.	1.5	30
33	DFT study of anatase-derived TiO2nanosheets/graphene hybrid materials. Physica Status Solidi (B): Basic Research, 2014, 251, 1471-1479.	0.7	29
34	Revealing the Chemistry between Band Gap and Binding Energy for Leadâ€/Tinâ€Based Trihalide Perovskite Solar Cell Semiconductors. ChemSusChem, 2018, 11, 449-463.	3.6	27
35	Phase evolution of electrochemically potassium intercalated graphite. Journal of Materials Chemistry A, 2021, 9, 11187-11200.	5.2	27
36	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.	1.5	26

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37	Carbonateâ€Promoted Catalytic Activity of Potassium Cations for Soot Combustion by Gaseous Oxygen. ChemCatChem, 2014, 6, 479-484.	1.8	26
38	First-principles study of fast Na diffusion in Na3P. Chemical Physics Letters, 2014, 612, 129-133.	1.2	26
39	Theoretical study on quantum control of photodissociation and photodesorption dynamics by femtosecond chirped laser pulses. Journal of Chemical Physics, 1999, 110, 7756-7769.	1.2	25
40	Ab initiotheory for current-induced molecular switching: Melamine on Cu(001). Physical Review B, 2013, 87, .	1.1	25
41	Excitons at the (001) surface of anatase: Spatial behavior and optical signatures. Physical Review B, 2011, 84, .	1.1	23
42	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.	6.6	23
43	STM and laser-driven atom switch: â€,An open-system density-matrix study of H/Si(100). Physical Review B, 2003, 67, .	1.1	21
44	Parameterized Bases for Calculating Vibrational Spectra Directly from ab Initio Data Using Rectangular Collocation. Journal of Chemical Theory and Computation, 2012, 8, 2053-2061.	2.3	21
45	Revealing Factors Influencing the Fluorineâ€Centered Nonâ€Covalent Interactions in Some Fluorineâ€Substituted Molecular Complexes: Insights from Firstâ€Principles Studies. ChemPhysChem, 2018, 19, 1486-1499.	1.0	21
46	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.	1.0	20
47	Dynamic behavior of the IRC in chemical laser systems. Theoretica Chimica Acta, 1982, 60, 523-533.	0.9	19
48	First-Principle Calculations of Solvated Electrons at Protic Solventâ^'TiO₂ Interfaces with Oxygen Vacancies. Journal of Physical Chemistry C, 2009, 113, 7236-7245.	1.5	19
49	Redox Reaction Mechanisms with Non-triiodide Mediators in Dye-Sensitized Solar Cells by Redox Potential Calculations. Journal of Physical Chemistry Letters, 2012, 3, 3581-3584.	2.1	19
50	Role of Quantum-Confinement in Anatase Nanosheets. Journal of Physical Chemistry Letters, 2017, 8, 3867-3873.	2.1	19
51	Palladiumâ€Catalyzed Intramolecular Câ^'H Arylation versus 1,5â€Palladium Migration: A Theoretical Investigation. Chemistry - an Asian Journal, 2018, 13, 2566-2572.	1.7	19
52	Effects of vibrational relaxation on the photodesorption of NO from Pt(111): A density matrix study. Journal of Chemical Physics, 2003, 119, 9710-9718.	1.2	17
53	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, 1487.	1.7	17
54	Charge Storage Mechanism of RuO₂/Water Interfaces. Journal of Physical Chemistry C, 2017, 121, 18975-18981.	1.5	15

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55	of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mo stretchy="false">(</mml:mo><mml:mi>Ga</mml:mi><mml:mrow><mml:mrow><mml:mi) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf		

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73	ChalcogenÂ·Â·Â·Chalcogen Bonding in Molybdenum Disulfide, Molybdenum Diselenide and Molybdenum Ditelluride Dimers as Prototypes for a Basic Understanding of the Local Interfacial Chemical Bonding Environment in 2D Layered Transition Metal Dichalcogenides. Inorganics, 2022, 10, 11.	1.2	8
74	A theoretical study of molecular conduction. V. NEGFâ€based MP2 approach. International Journal of Quantum Chemistry, 2009, 109, 1834-1840.	1.0	7
75	First-principles study of electronic structure and charge transport at PTCDA molecular layers on Ag(111) and Al(111) electrodes. Physical Review B, 2011, 84, .	1.1	7
76	Energy Alignment of Frontier Orbitals and Suppression of Charge Recombinations in P3HT/SWNT. Journal of Physical Chemistry C, 2015, 119, 26258-26265.	1.5	7
77	Dipole analyses for short-circuit current in organic photovoltaic devices of diketopyrrolopyrrole-based donor and PCBM. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	6
78	Theoretical study of molecular conduction: I. Effective Green's function based on perturbation theory. International Journal of Quantum Chemistry, 2006, 106, 803-813.	1.0	4
79	Effect of Isotopic Substitution on Elementary Processes in Dye-Sensitized Solar Cells: Deuterated Amino-Phenyl Acid Dyes on TiO2. Computation, 2013, 1, 1-15.	1.0	4
80	Electron wavepacket approaches to non-adiabatic transition processes in the internal rotational motion of H2CNH2+ â€“ Charge oscillation due to electronic coherence. Chemical Physics Letters, 2015, 635, 345-349.	1.2	4
81	Theoretical Verification of Photoelectrochemical Water Oxidation Using Nanocrystalline TiO2 Electrodes. Molecules, 2015, 20, 9732-9744.	1.7	4
82	A Theoretical study on the charge and discharge states of Naâ€ion battery cathode material, Na_{1+x}FePO₄F. Journal of Computational Chemistry, 2019, 40, 237-246.	1.5	4
83	Semiclassical quantization of nonadiabatic systems with hopping periodic orbits. Journal of Chemical Physics, 2015, 142, 074104.	1.2	3
84	Post-lithium-ion batteries: characterization of phosphorous and tin for potassium-ion anodes. Journal of Materials Science, 2021, 56, 10926-10937.	1.7	3
85	First-principle Calculations of Dopant-Oxygen Vacancy Complexes in Transparent Conducting TiO2 Systems. Hyomen Kagaku, 2010, 31, 343-351.	0.0	3
86	A new implementation of ab initio ehrenfest dynamics using electronic configuration basis: Exact formulation with molecular orbital connection and effective propagation scheme with locally quasiâ€diabatic representation. International Journal of Quantum Chemistry, 2016, 116, 1205-1213.	1.0	2
87	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.	1.0	2
88	Halogen in materials design: Chloroammonium lead triiodide perovskite (ClNH 3 PbI 3) a dynamical bandgap semiconductor in 3D for photovoltaics. Journal of Computational Chemistry, 2018, 39, 1902-1912.	1.5	2
89	A theoretical study on quantum control of photodissociation dynamics by ultrashort chirped laser pulses. International Journal of Quantum Chemistry, 1999, 72, 525-532.	1.0	1
90	Absorption spectra of alkali atoms (Li,â€ŠNa,â€ŠK) attached to superfluid helium clusters: A path integral Monte Carlo study. AIP Conference Proceedings, 2001, , .	0.3	1

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91	Local Electronic Excitation Mechanism for Nanofabrication of Polydiacetylene Molecular Wire. Journal of the Physical Society of Japan, 2003, 72, 3286-3290.	0.7	1
92	Computational DFT Study of ZrSiO4 Polymorphs: Microelectronic, Nuclear Safety and Geological Implications. Materials Research Society Symposia Proceedings, 2005, 894, 1.	0.1	1
93	A THEORETICAL STUDY OF POINT DEFECTS IN ZIRCONIA â€“ SILICON INTERFACES. International Journal of High Speed Electronics and Systems, 2006, 16, 389-396.	0.3	1
94	Theoretical Studies of Solvation Effects on 2-(2-Hydroxyphenyl)benzimidazole. Chemistry Letters, 2012, 41, 672-673.	0.7	1
95	Theoretical Study of Surface Complexes between TiO2 and HeteroTCNQs Showing Interfacial Charge-Transfer Transitions Designed Based on Redox Potential. Bulletin of the Chemical Society of Japan, 2015, 88, 1410-1416.	2.0	1
96	Electronic and Optical Properties of Low-Dimensional TiO2: From Minority Surfaces to Nanocomposites. ACS Symposium Series, 2015, , 47-80.	0.5	1
97	Theoretical investigation of [Ru(tpy)2]2+, [Ru(tpy)(bpy)(H₂O)]2+ and [Ru(tpy)(bpy)(Cl)]+ complexes in acetone revisited: Inclusion of strong spinâ€“orbit couplings to quantum chemistry calculations. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650001.	1.8	1
98	Importance of Side-Chains on Molecular Characteristics of Interacting Organic Molecules. ACS Omega, 2019, 4, 10396-10404.	1.6	1
99	Laser-induced fluorescence of the CHFCHO radical and reaction of OH radicals with halogenated ethylenes. Journal of Chemical Physics, 2019, 150, 174302.	1.2	1
100	Electric Field Effects on Proton Transfer Reactions at Metal Electrodes: A DFT Study on H⁺(H₂O)₂/Pt(111) and Ag(111). Electrochemistry, 1999, 67, 1214-1217.	0.6	1
101	Control of Chemical Reactions by Using Chirped Laser Pulses. ACS Symposium Series, 2002, , 81-97.	0.5	0
102	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	0
103	The intrinsic reaction coordinate approach in polyatomic reaction dynamics. International Journal of Quantum Chemistry, 2009, 24, 177-189.	1.0	0
104	Modeling and Simulation of Photocatalytic Reactions at TiO2 Surfaces. , 0, , 37-75.		0
105	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.	0.5	0
106	DFT study of anatase-derived TiO2nanosheets/graphene hybrid materials (Phys. Status Solidi B 8/2014). Physica Status Solidi (B): Basic Research, 2014, 251, n/a-n/a.	0.7	0
107	Ab Initio Study of Internal Conversion through S1/S2 and S2/S3 Conical Intersections of 6-Acetyl-2-(N,N-dimethylamino)naphthalene. Chemistry Letters, 2015, 44, 1753-1755.	0.7	0
108	Quantum-classical correspondence in steady states of nonadiabatic systems. AIP Conference Proceedings, 2015, , .	0.3	0

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109	Laser-induced fluorescence of the trans-CHBrCHO radical. Journal of Chemical Physics, 2020, 153, 104301.	1.2	0
110	Decoherence of Entanglement in Markov Approximation in Terms of Rotating Wave Approximation. Journal of Computer Chemistry Japan, 2012, 11, 17-23.	0.0	0
111	Electronic and Optical Properties of Nitrogen-Doped Layered Manganese Oxides. Ceramic Transactions, 0, , 135-140.	0.1	0
112	Charge Separation and Charge Carrier Trapping of Lead Iodide Perovskites. , 0, , .		0
113	Effects of Titania Coatings on Hydrodesulfurization Catalysts: Insights from First-principles Calculations. Journal of the Japan Petroleum Institute, 2018, 61, 288-293.	0.4	0