

# Koichi Yamashita

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	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.. <i>International Journal of Molecular Sciences</i> , <b>2022</b> , 23,	6.3	5
107	Chalcogen-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. <i>Inorganics</i> , <b>2022</b> , 10, 11	2.9	4
106	The Phosphorus Bond, or the Phosphorus-Centered Pnictogen Bond: The Covalently Bound Phosphorus Atom in Molecular Entities and Crystals as a Pnictogen Bond Donor.. <i>Molecules</i> , <b>2022</b> , 27,	4.8	3
105	The Nitrogen Bond, or the Nitrogen-Centered Pnictogen Bond: The Covalently Bound Nitrogen Atom in Molecular Entities and Crystals as a Pnictogen Bond Donor. <i>Compounds</i> , <b>2022</b> , 2, 80-110		3
104	Post-lithium-ion batteries: characterization of phosphorous and tin for potassium-ion anodes. <i>Journal of Materials Science</i> , <b>2021</b> , 56, 10926-10937	4.3	1
103	Phase evolution of electrochemically potassium intercalated graphite. <i>Journal of Materials Chemistry A</i> , <b>2021</b> , 9, 11187-11200	13	9
102	Unveiling charge dynamics of visible light absorbing oxysulfide for efficient overall water splitting. <i>Nature Communications</i> , <b>2021</b> , 12, 7055	17.4	4
101	Laser-induced fluorescence of the trans-CHBrCHO radical. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 104301,9	3.9	1
100	Laser-induced fluorescence of the CHFCHO radical and reaction of OH radicals with halogenated ethylenes. <i>Journal of Chemical Physics</i> , <b>2019</b> , 150, 174302	3.9	1
99	Importance of Side-Chains on Molecular Characteristics of Interacting Organic Molecules. <i>ACS Omega</i> , <b>2019</b> , 4, 10396-10404	3.9	
98	Li and Na Interaction with Ti2C-MXene: A First-Principles Calculation. <i>Journal of Computer Chemistry Japan</i> , <b>2019</b> , 18, 84-94	0.2	8
97	Significance of hydrogen bonding and other noncovalent interactions in determining octahedral tilting in the CHNHPbI hybrid organic-inorganic halide perovskite solar cell semiconductor. <i>Scientific Reports</i> , <b>2019</b> , 9, 50	4.9	57
96	A Theoretical study on the charge and discharge states of Na-ion battery cathode material, Na FePO F. <i>Journal of Computational Chemistry</i> , <b>2019</b> , 40, 237-246	3.5	1
95	Molecular QTAIM Topology Is Sensitive to Relativistic Corrections. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 2538-2544	4.8	9
94	Revealing Factors Influencing the Fluorine-Centered Non-Covalent Interactions in Some Fluorine-Substituted Molecular Complexes: Insights from First-Principles Studies. <i>ChemPhysChem</i> , <b>2018</b> , 19, 1486-1499	3.2	16
93	Halogen in materials design: Fluoroammonium lead triiodide (FNH3PbI3) perovskite as a newly discovered dynamical bandgap semiconductor in 3D. <i>International Journal of Quantum Chemistry</i> , <b>2018</b> , 118, e25621	2.1	1
92	Palladium-Catalyzed Intramolecular C-H Arylation versus 1,5-Palladium Migration: A Theoretical Investigation. <i>Chemistry - an Asian Journal</i> , <b>2018</b> , 13, 2566-2572	4.5	14

91	Effects of Titania Coatings on Hydrodesulfurization Catalysts: Insights from First-principles Calculations. <i>Journal of the Japan Petroleum Institute</i> , <b>2018</b> , 61, 288-293	1	
90	Do surfaces of positive electrostatic potential on different halogen derivatives in molecules attract? like attracting like!. <i>Journal of Computational Chemistry</i> , <b>2018</b> , 39, 343-350	3.5	24
89	Revealing the Chemistry between Band Gap and Binding Energy for Lead-/Tin-Based Trihalide Perovskite Solar Cell Semiconductors. <i>ChemSusChem</i> , <b>2018</b> , 11, 449-463	8.3	22
88	Halogen in materials design: Chloroammonium lead triiodide perovskite (ClNH PbI <sub>3</sub> ) a dynamical bandgap semiconductor in 3D for photovoltaics. <i>Journal of Computational Chemistry</i> , <b>2018</b> , 39, 1902-1912	3.5	2
87	Nature of the Electronic and Optical Excitations of Ruddlesden-Popper Hybrid Organic-Inorganic Perovskites: The Role of the Many-Body Interactions. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 5891-5896	6.4	38
86	Can Combined Electrostatic and Polarization Effects Alone Explain the F <sup>−</sup> F <sup>−</sup> Negative-Negative Bonding in Simple Fluoro-Substituted Benzene Derivatives? A First-Principles Perspective. <i>Computation</i> , <b>2018</b> , 6, 51	2.2	21
85	Epitaxy of (GaN) <sub>1-x</sub> (ZnO) <sub>x</sub> Solid-Solution Thin Films with Widely Tunable Chemical Composition and Strong Visible Absorption. <i>Physical Review Applied</i> , <b>2018</b> , 10,	4.3	9
84	Two-dimensional optical excitations in the mixed-valence Cs <sub>2</sub> Au <sub>2</sub> I <sub>6</sub> fully inorganic double perovskite. <i>Journal of Materials Chemistry C</i> , <b>2018</b> , 6, 10197-10201	7.1	20
83	Influence of the aggregate state on band structure and optical properties of C <sub>60</sub> computed with different methods. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 204301	3.9	9
82	-1 Isomers of tethered bismethano[70]fullerene as electron acceptors in organic photovoltaics.. <i>RSC Advances</i> , <b>2018</b> , 8, 18316-18326	3.7	9
81	Revealing the Cooperative Chemistry of the Organic Cation in the Methylammonium Lead Triiodide Perovskite Semiconductor System. <i>ChemistrySelect</i> , <b>2018</b> , 3, 7269-7282	1.8	6
80	Development of a Classical Interatomic Potential for MAPbBr <sub>3</sub> . <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 3724-3733	3.8	19
79	Charge Carrier Trapping at Surface Defects of Perovskite Solar Cell Absorbers: A First-Principles Study. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 742-746	6.4	181
78	Synthesis of Quinoidal Fused Oligosiloles by Rhodium-Catalyzed Stitching Reaction and Theoretical Investigation of Their Properties. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 3861-3867	16.4	20
77	First-Principles Study of the Band Diagrams and Schottky-Type Barrier Heights of Aqueous TaN Interfaces. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2017</b> , 9, 9559-9566	9.5	8
76	Defects in crystalline PVDF: a density functional theory-density functional tight binding study. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 7560-7567	3.6	5
75	Charge Storage Mechanism of RuO <sub>2</sub> /Water Interfaces. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 18975-18981	3.1	10
74	Hybrid organic-inorganic CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> perovskite building blocks: Revealing ultra-strong hydrogen bonding and mulliken inner complexes and their implications in materials design. <i>Journal of Computational Chemistry</i> , <b>2017</b> , 38, 2802-2818	3.5	23

73	Role of Quantum-Confinement in Anatase Nanosheets. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 3867-3873	6.4	17
72	Inorganic Lattice Fluctuation Induces Charge Separation in Lead Iodide Perovskites: Theoretical Insights. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 26648-26654	3.8	8
71	Zero-Dimensional Hybrid Organic-Inorganic Halide Perovskite Modeling: Insights from First Principles. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 888-99	6.4	35
70	Black Phosphorus as a High-Capacity, High-Capability Negative Electrode for Sodium-Ion Batteries: Investigation of the Electrode/Electrolyte Interface. <i>Chemistry of Materials</i> , <b>2016</b> , 28, 1625-1635	9.6	199
69	Theoretical investigation of [Ru(tpy) <sub>2</sub> ] <sup>2+</sup> , [Ru(tpy)(bpy)(H <sub>2</sub> O)] <sup>2+</sup> and [Ru(tpy)(bpy)(Cl)] <sup>+</sup> complexes in acetone revisited: Inclusion of strong spin-orbit couplings to quantum chemistry calculations. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2016</b> , 15, 1650001	1.8	0
68	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. <i>International Journal of Quantum Chemistry</i> , <b>2016</b> , 116, 1205-1213	2.1	2
67	Remarkable Dependence of the Final Charge Separation Efficiency on the Donor-Acceptor Interaction in Photoinduced Electron Transfer. <i>Angewandte Chemie - International Edition</i> , <b>2016</b> , 55, 629-334	16.4	79
66	The Effects of the Organic-Inorganic Interactions on the Thermal Transport Properties of CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> . <i>Nano Letters</i> , <b>2016</b> , 16, 2749-53	11.5	80
65	Atomic-Scale Analysis of the RuO <sub>2</sub> /Water Interface under Electrochemical Conditions. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 8096-8103	3.8	35
64	Dipole analyses for short-circuit current in organic photovoltaic devices of diketopyrrolopyrrole-based donor and PCBM. <i>Theoretical Chemistry Accounts</i> , <b>2016</b> , 135, 1	1.9	5
63	Thermal effect on the morphology and performance of organic photovoltaics. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 26456-26465	3.6	8
62	The mechanism of slow hot-hole cooling in lead-iodide perovskite: first-principles calculation on carrier lifetime from electron-phonon interaction. <i>Nano Letters</i> , <b>2015</b> , 15, 3103-8	11.5	121
61	Electronic and Optical Properties of Low-Dimensional TiO <sub>2</sub> : From Minority Surfaces to Nanocomposites. <i>ACS Symposium Series</i> , <b>2015</b> , 47-80	0.4	1
60	Semiclassical quantization of nonadiabatic systems with hopping periodic orbits. <i>Journal of Chemical Physics</i> , <b>2015</b> , 142, 074104	3.9	3
59	Organic-inorganic halide perovskites: an ambipolar class of materials with enhanced photovoltaic performances. <i>Journal of Materials Chemistry A</i> , <b>2015</b> , 3, 8981-8991	13	89
58	Theoretical Study of Surface Complexes between TiO <sub>2</sub> and Heteroatom TCNQs Showing Interfacial Charge-Transfer Transitions Designed Based on Redox Potential. <i>Bulletin of the Chemical Society of Japan</i> , <b>2015</b> , 88, 1410-1416	5.1	1
57	Alternative, Lead-free, Hybrid Organic-Inorganic Perovskites for Solar Applications: A DFT Analysis. <i>Chemistry Letters</i> , <b>2015</b> , 44, 826-828	1.7	60
56	Ab Initio Study of Internal Conversion through S <sub>1</sub> /S <sub>2</sub> and S <sub>2</sub> /S <sub>3</sub> Conical Intersections of 6-Acetyl-2-(N,N-dimethylamino)naphthalene. <i>Chemistry Letters</i> , <b>2015</b> , 44, 1753-1755	1.7	

55	Electron wavepacket approaches to non-adiabatic transition processes in the internal rotational motion of H <sub>2</sub> CNH <sub>2</sub> <sup>+</sup> [Charge oscillation due to electronic coherence. <i>Chemical Physics Letters</i> , <b>2015</b> , 635, 345-349	2.5	4
54	A density functional tight binding study of acetic acid adsorption on crystalline and amorphous surfaces of titania. <i>Molecules</i> , <b>2015</b> , 20, 3371-88	4.8	33
53	Theoretical Verification of Photoelectrochemical Water Oxidation Using Nanocrystalline TiO <sub>2</sub> Electrodes. <i>Molecules</i> , <b>2015</b> , 20, 9732-44	4.8	3
52	Energy Alignment of Frontier Orbitals and Suppression of Charge Recombinations in P3HT/SWNT. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 26258-26265	3.8	7
51	Organic-Inorganic Hybrid Lead Iodide Perovskite Featuring Zero Dipole Moment Guanidinium Cations: A Theoretical Analysis. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 4694-4701	3.8	108
50	Electronic Schrödinger equation with nonclassical nuclei. <i>Physical Review A</i> , <b>2014</b> , 89,	2.6	37
49	First-principles study of fast Na diffusion in Na <sub>3</sub> P. <i>Chemical Physics Letters</i> , <b>2014</b> , 612, 129-133	2.5	24
48	DFT study of anatase-derived TiO <sub>2</sub> nanosheets/graphene hybrid materials. <i>Physica Status Solidi (B): Basic Research</i> , <b>2014</b> , 251, 1471-1479	1.3	23
47	Penetration Barrier of Water through Graphynes Pores: First-Principles Predictions and Force Field Optimization. <i>Journal of Physical Chemistry Letters</i> , <b>2014</b> , 5, 751-5	6.4	66
46	Electron-electron and electron-phonon correlation effects on the finite-temperature electronic and optical properties of zinc-blende GaN. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	38
45	Comparative Study of Sodium and Lithium Intercalation and Diffusion Mechanism in Black Phosphorus from First-principles Simulation. <i>Chemistry Letters</i> , <b>2014</b> , 43, 1940-1942	1.7	36
44	Carbonate-Promoted Catalytic Activity of Potassium Cations for Soot Combustion by Gaseous Oxygen. <i>ChemCatChem</i> , <b>2014</b> , 6, 479-484	5.2	24
43	The proton conduction mechanism in a material consisting of packed acids. <i>Chemical Science</i> , <b>2014</b> , 5, 4878-4887	9.4	55
42	Small Photocarrier Effective Masses Featuring Ambipolar Transport in Methylammonium Lead Iodide Perovskite: A Density Functional Analysis. <i>Journal of Physical Chemistry Letters</i> , <b>2013</b> , 4, 4213-6	6.4	543
41	Ab initio theory for current-induced molecular switching: Melamine on Cu(001). <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	24
40	Effect of Isotopic Substitution on Elementary Processes in Dye-Sensitized Solar Cells: Deuterated Amino-Phenyl Acid Dyes on TiO <sub>2</sub> . <i>Computation</i> , <b>2013</b> , 1, 1-15	2.2	4
39	Theoretical Studies of Solvation Effects on 2-(2-Hydroxyphenyl)benzimidazole. <i>Chemistry Letters</i> , <b>2012</b> , 41, 672-673	1.7	1
38	Electron trapping at the lattice Ti atoms adjacent to the Nb dopant in Nb-doped rutile TiO <sub>2</sub> . <i>Journal of Materials Science</i> , <b>2012</b> , 47, 7522-7529	4.3	9

37	Redox Reaction Mechanisms with Non-triiodide Mediators in Dye-Sensitized Solar Cells by Redox Potential Calculations. <i>Journal of Physical Chemistry Letters</i> , <b>2012</b> , 3, 3581-4	6.4	18
36	Parameterized Bases for Calculating Vibrational Spectra Directly from ab Initio Data Using Rectangular Collocation. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 2053-61	6.4	16
35	Towards Accurate Spectroscopic Identification of Species at Catalytic Surfaces: Anharmonic Vibrations of Formate on AuPt. <i>Materials Research Society Symposia Proceedings</i> , <b>2012</b> , 1484, 1		9
34	Decoherence of Entanglement in Markov Approximation in Terms of Rotating Wave Approximation. <i>Journal of Computer Chemistry Japan</i> , <b>2012</b> , 11, 17-23	0.2	
33	Theoretical Study of the Surface Complex between TiO <sub>2</sub> and TCNQ Showing Interfacial Charge-Transfer Transitions. <i>Journal of Physical Chemistry Letters</i> , <b>2011</b> , 2, 1167-70	6.4	81
32	Excitons at the (001) surface of anatase: Spatial behavior and optical signatures. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	21
31	Theoretical studies on a new pattern of laser-driven systems: towards elucidation of direct photo-injection in dye-sensitized solar cells. <i>Theoretical Chemistry Accounts</i> , <b>2011</b> , 130, 227-236	1.9	
30	Nonspectral Methods for Solving the Schrödinger Equation for Electronic and Vibrational Problems. <i>Journal of Physical Chemistry Letters</i> , <b>2011</b> , 2, 2193-2199	6.4	8
29	First-principles study of electronic structure and charge transport at PTCDA molecular layers on Ag(111) and Al(111) electrodes. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	7
28	Theoretical Studies on Proton Transfer among a High Density of Acid Groups: Surface of Zirconium Phosphate with Adsorbed Water Molecules. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 5599-5606	3.8	21
27	Theoretical and Experimental Studies on Reaction Mechanism for Aerobic Alcohol Oxidation by Supported Ruthenium Hydroxide Catalysts. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 10873-10880	3.8	29
26	First-principle Calculations of Dopant-Oxygen Vacancy Complexes in Transparent Conducting TiO <sub>2</sub> Systems. <i>Hyomen Kagaku</i> , <b>2010</b> , 31, 343-351		3
25	The intrinsic reaction coordinate approach in polyatomic reaction dynamics. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 24, 177-189	2.1	
24	A theoretical study of molecular conduction. V. NEGF-based MP2 approach. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 109, 1834-1840	2.1	7
23	First-Principle Calculations of Solvated Electrons at Protic Solvent/TiO <sub>2</sub> Interfaces with Oxygen Vacancies. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 7236-7245	3.8	17
22	Model calculation of the electron-phonon coupling in Cs/Cu(111). <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	8
21	A THEORETICAL STUDY OF POINT DEFECTS IN ZIRCONIA/SILICON INTERFACES. <i>International Journal of High Speed Electronics and Systems</i> , <b>2006</b> , 16, 389-396	0.5	1
20	Theoretical study of molecular conduction: I. Effective Green's function based on perturbation theory. <i>International Journal of Quantum Chemistry</i> , <b>2006</b> , 106, 803-813	2.1	4

19	Computational DFT Study of ZrSiO <sub>4</sub> Polymorphs: Potential Microelectronic, Nuclear Safety and Geological Implications. <i>Materials Research Society Symposia Proceedings</i> , <b>2005</b> , 894, 1		1
18	A FLUX-FLUX CROSS-CORRELATION FUNCTION APPROACH TO SELF-DIFFUSION OF HYDROGEN ATOM ON A CU(111) SURFACE. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2005</b> , 04, 209-223	1.8	
17	Local Electronic Excitation Mechanism for Nanofabrication of Polydiacetylene Molecular Wire. <i>Journal of the Physical Society of Japan</i> , <b>2003</b> , 72, 3286-3290	1.5	1
16	STM and laser-driven atom switch: An open-system density-matrix study of H/Si(100). <i>Physical Review B</i> , <b>2003</b> , 67,	3.3	20
15	Quantum chemical calculations on Al-CVD using DMEAA: surface reaction mechanism of AlH <sub>3</sub> on Al(111). <i>Molecular Physics</i> , <b>2003</b> , 101, 267-276	1.7	9
14	Effects of vibrational relaxation on the photodesorption of NO from Pt(111): A density matrix study. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 9710-9718	3.9	16
13	Control of Chemical Reactions by Using Chirped Laser Pulses. <i>ACS Symposium Series</i> , <b>2002</b> , 81-97	0.4	
12	Theoretical study on the structure of Na <sup>+</sup> -doped helium clusters: Path integral Monte Carlo calculations. <i>Journal of Chemical Physics</i> , <b>2000</b> , 112, 10966-10975	3.9	51
11	Theoretical study on quantum control of photodissociation and photodesorption dynamics by femtosecond chirped laser pulses. <i>Journal of Chemical Physics</i> , <b>1999</b> , 110, 7756-7769	3.9	24
10	Theoretical studies of the potential energy surface and wavepacket dynamics of the Li <sub>3</sub> system. <i>Theoretical Chemistry Accounts</i> , <b>1999</b> , 102, 226-236	1.9	6
9	A theoretical study on quantum control of photodissociation dynamics by ultrashort chirped laser pulses. <i>International Journal of Quantum Chemistry</i> , <b>1999</b> , 72, 525-532	2.1	1
8	Electric Field Effects on Proton Transfer Reactions at Metal Electrodes: A DFT Study on H+(H <sub>2</sub> O) <sub>2</sub> /Pt(111) and Ag(111). <i>Electrochemistry</i> , <b>1999</b> , 67, 1214-1217	1.2	1
7	A theoretical study on laser control of a molecular nonadiabatic process by ultrashort chirped laser pulses. <i>Journal of Chemical Physics</i> , <b>1998</b> , 109, 1801-1809	3.9	33
6	Theoretical study of the low-lying electronic states of XeO and XeS. <i>Journal of Chemical Physics</i> , <b>1998</b> , 108, 1514-1521	3.9	32
5	The dissociation of HNO. I. Potential energy surfaces for the X <sup>1</sup> A <sub>1</sub> , <sup>2</sup> A <sub>1</sub> , and <sup>2</sup> B <sub>1</sub> states. <i>Journal of Chemical Physics</i> , <b>1997</b> , 107, 6603-6615	3.9	34
4	Ab initio studies on the interstellar molecules C <sub>3</sub> H <sub>2</sub> and C <sub>3</sub> H and the mechanism for the neutral-neutral reaction C(3P)+C <sub>2</sub> H <sub>2</sub> . <i>Journal of Chemical Physics</i> , <b>1996</b> , 104, 6613-6627	3.9	68
3	Dynamic behavior of the IRC in chemical laser systems. <i>Theoretica Chimica Acta</i> , <b>1982</b> , 60, 523-533		18
2	Modeling and Simulation of Photocatalytic Reactions at TiO <sub>2</sub> Surfaces	37-75	

1 Electronic and Optical Properties of Nitrogen-Doped Layered Manganese Oxides. *Ceramic Transactions*,135-140

0.1