Kazuyoshi Ogasawara

List of Publications by Citations

110 papers	1,301 citations	19 h-index	32 g-index
119 ext. papers	1,414 ext. citations	2.5 avg, IF	4.3 L-index

#	Paper	IF	Citations
110	Relativistic cluster calculation of ligand-field multiplet effects on cation L2,3 x-ray-absorption edges of SrTiO3, NiO, and CaF2. *Physical Review B*, **2001**, 64,	3.3	146
109	Core-hole effects on theoretical electron-energy-loss near-edge structure and near-edge x-ray absorption fine structure of MgO. *Physical Review B*, **2000**, 61, 2180-2187	3.3	89
108	First-principles multielectron calculations of Ni L2,3 NEXAFS and ELNES for LiNiO2 and related compounds. *Physical Review B*, **2005**, 72,	3.3	86
107	Calculation of multiplet structures of Cr3+ and V3+ in Al2O3 based on a hybrid method of density-functional theory and the configuration interaction. *Physical Review B*, **2000**, 61, 143-161	3.3	70
106	First-principles calculations of electron-energy-loss near-edge structure and near-edge x-ray-absorption fine structure of BN polytypes using model clusters. *Physical Review B*, **1999**, 60, 4944-4951	3.3	55
105	First Principles Calculation of Fe L2,3-edge X-ray Absorption Near Edge Structures of Iron Oxides. *Materials Transactions*, **2004**, 45, 1414-1418	1.3	50
104	Optical spectra of trivalent lanthanides in LiYF4 crystal. *Journal of Solid State Chemistry*, **2005**, 178, 412-418	3.3	48
103	Fully relativistic calculations of the L2,3-edge XANES spectra for vanadium oxides. *European Physical Journal B*, **2006**, 51, 345-355	1.2	38
102	Microscopic analysis of the crystal field strength and lowest charge transfer energies in the elpasolite crystals Cs2NaYX6(X=F,Cl,Br) doped with Cr3+. *Physical Review B*, **2006**, 74,	3.3	35
101	Study of multiplet structures of Mn4+ activated in fluoride crystals. *Journal of Luminescence*, **2016**, 169, 594-600	3.8	31
100	Semiconductive Nature of Lead-Based Metal-Organic Frameworks with Three-Dimensionally Extended Sulfur Secondary Building Units. *Journal of the American Chemical Society*, **2020**, 142, 27-32	16.4	29
99	Theoretical calculation for the multiplet structure of the tetrahedrally coordinated Cr4+ in Y3Al5O12. *Journal of Chemical Physics*, **2001**, 115, 492-508	3.9	28
98	Calculations of Complete 4fnand 4fn-15d1Energy Level Schemes of Free Trivalent Rare-Earth Ions. *Japanese Journal of Applied Physics*, **2004**, 43, L611-L613	1.4	26
97	Multiplet Energy Level Diagrams for Cr3+and Mn4+in Oxides with OhSite Symmetry Based on First-Principles Calculations. *ECS Journal of Solid State Science and Technology*, **2016**, 5, R3191-R3196	2	25
96	Cluster calculation of oxygen K-edge electron-energy-loss near-edge structure of NiO. *Physical Review B*, **1998**, 58, 9693-9696	3.3	25
95	Optical Transitions near the Fundamental Absorption Edge and Electronic Structures of YAl3(BO3)4:Gd3+. *Japanese Journal of Applied Physics*, **2006**, 45, 146-151	1.4	22
94	Comparative Study of Absorption Spectra of V2+, Cr3+, and Mn4+in Al2O3Based on First-Principles Configuration Interaction Calculations. *Journal of the Physical Society of Japan*, **2012**, 81, 104709	1.5	21

93	First-principles relativistic calculation for 4f□5d transition energy of Ce3+ in various fluoride hosts. *Journal of Solid State Chemistry*, **2006**, 179, 2438-2442	3.3	20
92	First-principles calculations of 4f□5d optical absorption spectra in BaMgAl10O17:Eu. *Journal of Luminescence*, **2007**, 122-123, 104-106	3.8	19
91	First-principles analysis method for the f□ transitions of heavy metal ions. *Journal of Alloys and Compounds*, **2004**, 374, 18-21	5.7	19
90	A New Metallic Langmuir-Blodgett Film Formed with BO$_{bf 2}$-(MeO)$_{bf 2}$TCNQ, where BO is Bisethylenedioxytetrathiafulvalene and (MeO)2TCNQ is Dimethoxytetracyanoquinodimethane. *Japanese Journal of Applied Physics*, **1996**, 35, L571-L573	1.4	18
89	Vacuum referred binding energy of 3d transition metal ions for persistent and photostimulated luminescence phosphors of cerium-doped garnets. *Journal of Luminescence*, **2017**, 192, 371-375	3.8	16
88	Study on Multiplet Energies of V2+, Cr3+, and Mn4+ in MgO Host Crystal Based on First-Principles Calculations with Consideration of Lattice Relaxation. *Journal of the Physical Society of Japan*, **2014**, 83, 124707	1.5	16
87	First-principles and experimental analysis of fn□n□1d1 absorption spectra and multiplet energy levels of Pr3+, Nd3+, and U3+ in LiYF4. *Physical Review B*, **2010**, 81,	3.3	16
86	First-principles calculation of ground and excited-state absorption spectra of ruby and alexandrite considering lattice relaxation. *Physical Review B*, **2009**, 79,	3.3	16
85	First-principles analysis method for the multiplet structures of rare-earth ions in solids. *Journal of Alloys and Compounds*, **2004**, 380, 136-140	5.7	16
84	Relativistic Calculations of Complete 4fnEnergy Level Schemes of Free Trivalent Rare-Earth Ions. *Japanese Journal of Applied Physics*, **2005**, 44, 7488-7490	1.4	16
83	Structural study of the highly conductive tridecylmethylammonium-Au(dmit)2 Langmuir-Blodgett films. *Synthetic Metals*, **1995**, 74, 251-255	3.6	16
82	Percolation conduction in BO-C10TCNQ conductive Langmuir-Blodgett films. *Journal of Physics and Chemistry of Solids*, **1997**, 58, 39-49	3.9	15
81	First-principles Calculation of Transition-metal L2,3-edge Electron-energy-loss Near-edge structures Based on Direct Diagonalization of the Many-electron Hamiltonian. *Materials Transactions*, **2002**, 43, 1435-1438	1.3	15
80	Investigation of Ion Dependence of Electronic Structure for 3d3 Ions in Mg2TiO4 Based on First-Principles Calculations. *ECS Transactions*, **2013**, 50, 9-17	1	14
79	Crystal field analysis of energy level structure of LaF3:Eu3+. *Journal of Alloys and Compounds*, **2006**, 408-412, 753-756	5.7	13
78	Theoretical calculation for the multiplet structures of tetrahedrally coordinated Cr4+in silicate crystals. *Journal of Physics Condensed Matter*, **2001**, 13, 5757-5784	1.8	13
77	Chapter 231 First-principles calculations of transition spectra. *Fundamental Theories of Physics*, **2007**, 1-59	0.8	12
76	Relativistic many-electron calculations of Cr3+ L2,3-edge x ray absorption near-edge structures for Cr3+:□Al2O3 and □Cr2O3 and magnetic circular dichroism of Cr3+L2,3-edge x ray absorption near-edge structures for Cr3+:□Al2O3. *Journal of Applied Physics*, **2011**, 110, 123524	2.5	11

75	Experimental and Theoretical Investigations for Excitation Properties of Ba[sub 1-x]Eu[sub x]MgAl[sub 10]O[sub 17]. *Journal of the Electrochemical Society*, **2007**, 154, J196	3.9	11
74	Experimental and First-Principles Analysis of 4f□5d Absorption Spectrum for Ce3+ in LiYF4 Considering Lattice Relaxation. *Journal of the Physical Society of Japan*, **2008**, 77, 084702	1.5	10
73	Microscopic Analysis of 5d States Splitting and Charge Transfer Energies Dependence on Interionic Distance in Alkaline Earth Fluorides Doped with Light Trivalent Lanthanides. *Spectroscopy Letters*, **2007**, 40, 221-235	1.1	8
72	A First-Principles Investigation of the Crystal-Field and Racah Parameters of Transition Metal Ions: Cr3+ in Alumina. *ECS Journal of Solid State Science and Technology*, **2020**, 9, 016011	2	8
71	Comparative study of the absorption spectrum of Li2CaSiO4:Cr4+: First-principles fully relativistic and crystal field calculations. *Optical Materials*, **2007**, 30, 399-406	3.3	7
70	Fully relativistic analysis of the absorption spectra of Ca3Sc2Ge3O12:Ni2+. *Physica Status Solidi (B): Basic Research*, **2006**, 243, 2864-2873	1.3	7
69	First-principles analysis for the multiplet structures of tetrahedrally and octahedrally oxo-coordinated 3d2 and 3d3 transition metals. *Journal of Chemical Physics*, **2002**, 116, 471-479	3.9	7
68	Comparative Study of Multiplet Structures of Mn^{4+} in K$_{2}$SiF$_{6}$, K$_{2}$GeF$_{6}$, and K$_{2}$TiF$_{6}$ Based on First-Principles Configuration□Interaction Calculations. *Japanese Journal of Applied Physics*, **2012**, 51, 022604	1.4	6
67	Luminescence properties of YAl3(BO3)4:Gd3+ phosphors substituted with Sc3+ ions. *Journal of Luminescence*, **2007**, 122-123, 488-491	3.8	6
66	Many-electron theory for electronic transition process □ts importance in materials science. *Advances in Quantum Chemistry*, **2003**, 42, 1-22	1.4	6
65	Multiplet structures of tetrahedrally coordinated Cr4+ and Cr5+ in Y3Al5O12. *Applied Physics Letters*, **2001**, 78, 2154-2156	3.4	6
64	Calculation of Multiplet Structure of Ruby Using Explicit Effective Hamiltonian. *Materials Transactions, JIM*, **1999**, 40, 396-399		6
63	Ab-initiostudy on the absorption spectrum of color change sapphire based on first-principles calculations with considering lattice relaxation-effect. *IOP Conference Series: Materials Science and Engineering*, **2018**, 299, 012060	0.4	6
62	Current Situation and Future Development of Discrete Variational Multielectron Method. *Advances in Quantum Chemistry*, **2008**, 54, 297-314	1.4	5
61	First principles calculations of the L2,3-edge XANES spectra for V2O3. *Radiation Physics and Chemistry*, **2006**, 75, 1564-1570	2.5	5
60	First-principles analysis for the optical absorption spectra of metal ions in solids. *International Journal of Quantum Chemistry*, **2004**, 99, 488-494	2.1	5
59	Proton Spin Relaxation due to Localization in Weakly Disordered System of BO-C10TCNQ Complex. *Journal of the Physical Society of Japan*, **1998**, 67, 1556-1559	1.5	5
58	Systematic first-principles calculations of charge transfer transitions of trivalent rare earth ions in CaF2. *Journal of Luminescence*, **2019**, 214, 116542	3.8	4

57	Comparative Study on R-line and U-band Energies of Ruby Estimated from One-Electron and Many-Electron First-Principles Approaches. *Journal of Physics: Conference Series*, **2019**, 1179, 012104	0.3	4
56	Molecular orbital calculations of Eu-doped SrAl2O4 clusters. *Solid State Communications*, **2015**, 206, 42-46	1.6	4
55	Analysis of Core-Hole Effect in Cation L2,3-Edge of MgO, Al2O3 and SiO2 Based on DV-X Cluster Calculations. *Advances in Quantum Chemistry*, **1998**, 441-466	1.4	4
54	Non-empirical study on pressure dependence of ruby bond length. *Journal of Physics: Conference Series*, **2019**, 1402, 066005	0.3	4
53	Study on the Optical Luminescence Properties of Li2TiO3: Mn4+ and Cr3+. *Chemistry Letters*, **2021**, 50, 52-56	1.7	4
52	Systematic first-principles calculations of charge transfer transitions of transition metal ions (Sc3+, Ti3+, V3+, Cr3+, Mn3+, Fe3+) in Al2O3. *Optical Materials: X*, **2019**, 1, 100005	1.7	3
51	Enhance electron-correlation effect on the ruby multiplet energy dependence on pressure. *Optical Materials*, **2020**, 110, 110520	3.3	3
50	Lattice Relaxation Effects on the Multiplet Energies of Ruby Under Pressure using One-Electron Calculations. *IOP Conference Series: Materials Science and Engineering*, **2020**, 835, 012010	0.4	3
49	Synthesis, Crystal Structure, and DFT Calculation of a Dioxido-bridged Dinuclear Oxidomolybdenum(V) Complex with 2-(2-Aminoethyl)aminoethanethiol. *X-ray Structure Analysis Online*, **2017**, 33, 37-39	0.2	3
48	Luminescence properties of YAl3(BO3)4 substituted with Sc3+ ions. *Physica Status Solidi (A) Applications and Materials Science*, **2006**, 203, 2701-2704	1.6	3
47	First principles calculation of ELNES by LCAO methods. *Journal of Electron Microscopy*, **2002**, 51, S107-S112		3
46	Theoretical Calculation for Multiplet Structure of Chromium Ion Pair in Ruby. *Materials Transactions, JIM*, **1999**, 40, 416-419		3
45	Study on the molecular orbital energies of ruby under pressure. *Optical Materials*, **2020**, 109, 110375	3.3	3
44	Redox-Active Tin Metal-Organic Framework with a Thiolate-Based Ligand. *Inorganic Chemistry*, **2021**, 60, 12691-12695	5.1	3
43	Comparative study of Auger-free luminescence of Rb2ZnCl4 crystals between experiment and calculation. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2013**, 10, 993-996		2
42	Total cluster energy calculation of lithium ion conductors by the DV-X method. *International Journal of Quantum Chemistry*, **2009**, 109, 2658-2663	2.1	2
41	Fluorescence spectra of Pr3+ ions in phosphate materials calculated by the DVME method. *International Journal of Quantum Chemistry*, **2009**, 109, 2753-2757	2.1	2
40	First-principles calculation of magnetic circular dichroism of transition-metal L2,3-edge X-ray absorption near-edge structures. *International Journal of Quantum Chemistry*, **2009**, 109, 2672-2676	2.1	2

39	Mechanism of Luminescence Enhancement in Ca[sub 4]YO(BO[sub 3])[sub 3]:Eu[sup 3+] by Gd Substitution under Vacuum Ultraviolet Light Excitation. *Journal of the Electrochemical Society*, **2008**, 155, J335	3.9	2
38	The effect of intrinsic trigonal distortion on the multiplet structures of ruby and emerald. *Advances in Quantum Chemistry*, **2000**, 37, 97-110	1.4	2
37	High Resolution X-Ray Study on Anomalous Diffraction Peak Shift in Dimerized Langmuir-Blodgett Superlattice Films. *Journal of the Physical Society of Japan*, **1993**, 62, 3114-3126	1.5	2
36	Comparative Study of Multiplet Structures of Mn4+in K2SiF6, K2GeF6, and K2TiF6Based on First-Principles Configuration□Interaction Calculations. *Japanese Journal of Applied Physics*, **2012**, 51, 022604	1.4	2
35	Machine-Learning-Assisted Selective Synthesis of a Semiconductive Silver Thiolate Coordination Polymer with Segregated Paths for Holes and Electrons. *Angewandte Chemie - International Edition*, **2021**, 60, 23217-23224	16.4	2
34	Prediction of 4f2□4f15d1 transition energy of Pr3+ in fluorides based on first-principles calculations and machine learning. *IOP Conference Series: Materials Science and Engineering*, **2020**, 835, 012009	0.4	1
33	Systematic First-Principles Calculations of Charge Transfer Transitions of Transition Metal Ions (Sc3+, Ti3+, V3+, Cr3+, Mn3+, Fe3+) in □Al2O3 with Structural Optimization. *IOP Conference Series: Materials Science and Engineering*, **2020**, 835, 012005	0.4	1
32	Theoretical and Experimental Consideration of Valence Band X-ray Photoelectron Spectroscopy Spectra of Cr-Deficient MgCr2-xO4. *Japanese Journal of Applied Physics*, **2007**, 46, 4175-4178	1.4	1
31	Separation of the effects of charge transfer, covalency and electron correlations on the multiplet structure of ruby based on first-principles cluster calculations. *Advances in Quantum Chemistry*, **2000**, 37, 69-83	1.4	1
30	First-principles calculation for multiplet structure of emerald. *Advances in Quantum Chemistry*, **2000**, 37, 85-96	1.4	1
29	Unusual X-Ray Diffraction Vector Shift Observed in Heterogeneous Langmuir-Blodgett Multilayer Films. *Materials Research Society Symposia Proceedings*, **1992**, 247, 835		1
28	Atomic Size Effect in the X-Ray Diffraction for Partially Disordered One-Dimensional Molecular Superlattice. *Journal of the Physical Society of Japan*, **1994**, 63, 4260-4261	1.5	1
27	Effect of trivalent manganese substitution in □Al2O3 crystal on the absorption spectra based on first-principles calculations. *Journal of Physics: Conference Series*, **2019**, 1402, 066004	0.3	1
26	Synthesis, Crystal Structure, and Relativistic DV-X□Calculation of a □Oxido-□molybdato(VI)-bridged Dinuclear Oxidomolybdenum(V) Complex with 2-(3-Aminopropyl)aminoethanethiol. *X-ray Structure Analysis Online*, **2018**, 34, 19-21	0.2	1
25	Chromaticity coordinates of ruby based on first-principles calculation. *Optical Materials*, **2021**, 121, 111539	3.3	1
24	First-Principles calculations of the interconfigurational transition energies of 4f - 4f-15d of Ln3+ ions in LiYF4 and CaF2. *Optical Materials*, **2021**, 122, 111656	3.3	0
23	A non-empirical lattice-relaxation estimation of TM3+ doped □Al2O3. *IOP Conference Series: Materials Science and Engineering*, **2020**, 850, 012029	0.4	0
22	Photoconductive Coordination Polymer with a Lead-Sulfur Two-Dimensional Coordination Sheet Structure. *Inorganic Chemistry*, **2021**, 60, 5436-5441	5.1	0

21	The DV-Xα Molecular Orbital Calculation Method and Recent Development **2015**, 3-23	
20	Optimization of first-principles calculation conditions for multiplet energies of Fe3 + and Co3 + in α-Al2O3. *IOP Conference Series: Materials Science and Engineering*, **2020**, 835, 012007	0.4
19	The magnetism change by Jahn-Teller distortionin octahedral hexa-coordinate complex. *IOP Conference Series: Materials Science and Engineering*, **2020**, 835, 012014	0.4
18	Recent applications of discrete variational multi-electron method. *IOP Conference Series: Materials Science and Engineering*, **2020**, 835, 012028	0.4
17	Optical properties of Co3+ doped in α-Al2O3 with Considering Lattice Relaxation Effect. *IOP Conference Series: Materials Science and Engineering*, **2020**, 835, 012011	0.4
16	Electronic states of Nd3+ ions in phosphate glasses calculated by the discrete-variational multi-electron method. *Journal of Non-Crystalline Solids*, **2010**, 356, 2454-2457	3.9
15	A new highly conductive BO-(MeO)2 TCNQ Langmuir-Blodgett film. *Synthetic Metals*, **1997**, 86, 1835-1836	3.6
14	P-202L: Late-News Poster: Luminescence and Excitation Properties of Host Lattice and Eu2+ Ions in BaMgAl10O17:Eu2+ Phosphor. *Digest of Technical Papers SID International Symposium*, **2007**, 38, 526-529	0.5
13	First-principles calculations of the V3+ absorption spectra in LiAlO2 and LiGaO2. *Journal of Non-Crystalline Solids*, **2006**, 352, 2376-2379	3.9
12	P-92: Luminescence Properties of YAl3(BO3)4: Tb3+ Phosphors Substituted with Sc3+ Ions under VUV Excitation. *Digest of Technical Papers SID International Symposium*, **2006**, 37, 550	0.5
11	Many-electron calculation for the analysis of optical absorption spectra in Cr4+-doped solid-state laser crystals. *Advances in Quantum Chemistry*, **2003**, 42, 67-76	1.4
10	FIRST-PRINCIPLES CALCULATION OF MULTIPLETS OF TRANSITION-METAL IONS IN CRYSTALS BASED ON DENSITY FUNCTIONAL METHOD. *Recent Advances in Computational*, **2002**, 278-292	
9	Localization effects in nuclear spin relaxation of a charge-transfer complex. *Synthetic Metals*, **1999**, 102, 1689-1690	3.6
8	First-Principles Study of the Crystal-Field and Racah Parameters of Cr3+ in Alumina. *ECS Meeting Abstracts*, **2020**, MA2020-02, 2735-2735	0
7	First-Principles Calculations of Charge Transfer Transitions of Eu3+ in Y2O3 and Y2O2S. *ECS Journal of Solid State Science and Technology*, **2020**, 9, 066005	2
6	Optical Materials. *Springer Series in Materials Science*, **2006**, 129-145	0.9
5	Comparative Study on Optical Properties of YPO4: Mn, Zr Phosphor by Experiment and Calculation **2015**, 217-235	
4	Effect of Molecular Distortion of Ligand Field Splitting in Five-Coordinated Metal Complex. *IOP Conference Series: Materials Science and Engineering*, **2020**, 835, 012022	0.4

3	Prediction of emission energy of Cr3+ in oxides based on first-principles calculations and machine learning. *IOP Conference Series: Materials Science and Engineering*, **2020**, 835, 012018	0.4
2	Mechanism of Optical Rotation of Amino Acids Using Electronic State Calculation. *IOP Conference Series: Materials Science and Engineering*, **2020**, 835, 012020	0.4
1	Machine-Learning-Assisted Selective Synthesis of a Semiconductive Silver Thiolate Coordination Polymer with Segregated Paths for Holes and Electrons. *Angewandte Chemie*, **2021**, 133, 23405	3.6