Isao Tanaka

List of Publications by Year in Descending Order

412 papers	19,886 citations	57 h-index	133 g-index
424 ext. papers	23,655 ext. citations	3.7 avg, IF	7.44 L-index

#	Paper	IF	Citations
412	Influence of Se doping on recently synthesized NaInS2-xSex solid solutions for potential thermo-mechanical applications studied via first-principles method. *Materials Today Communications*, **2021**, 26, 101988	2.5	5
411	Protonic Conduction in the BaNdInO Structure Achieved by Acceptor Doping. *Chemistry of Materials* , **2021**, 33, 2139-2146	9.6	9
410	Combination of recommender system and single-particle diagnosis for accelerated discovery of novel nitrides. *Journal of Chemical Physics*, **2021**, 154, 224117	3.9	1
409	Growth and characterization of Li7La3Zr2O12 single crystals by using floating zone method for use as fast Li-ion conductor *Journal of Physics: Conference Series*, **2021**, 1718, 012012	0.3	
408	NaInX2 (X = S, Se) layered materials for energy harvesting applications: first-principles insights into optoelectronic and thermoelectric properties. *Journal of Materials Science: Materials in Electronics*, **2021**, 32, 3878-3893	2.1	4
407	Effect of Li concentration on the ionic conductivity of LixLa(1)/3Nb0.80Ta0.20O3 solid solutions. *Journal of the Ceramic Society of Japan*, **2021**, 129, 535-539	1	
406	Cooperative Oxide-Ion Transport in Pyrochlore Y2Ti2O7: A First-Principles Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2021**, 125, 20460-20467	3.8	0
405	Investigating the combined effects of mirror tilting and position on rutile crystal growth using the infrared convergent-heating floating zone method. *Journal of Crystal Growth*, **2021**, 571, 126257	1.6	
404	Fluorine solubility and superconducting properties of Sm(O,F)BiS2 single crystals. *Journal of Alloys and Compounds*, **2021**, 883, 160812	5.7	
403	Lithium-ionic conductivity of LixLa(1)/3NbO3 single crystals grown by the TSFZ method. *Solid State Ionics*, **2020**, 350, 115330	3.3	3
402	Fast material search of lithium ion conducting oxides using a recommender system. *Journal of Materials Chemistry A*, **2020**, 8, 11582-11588	13	11
401	Growth of Cr2N single crystals by the floating zone method. *Journal of Crystal Growth*, **2020**, 546, 125782	1.6	1
400	Growth and Characterization of ROBiS High-Entropy Superconducting Single Crystals. *ACS Omega*, **2020**, 5, 16819-16825	3.9	4
399	Flux Growth and Superconducting Properties of (Ce,Pr)OBiS Single Crystals. *Frontiers in Chemistry*, **2020**, 8, 44	5	6
398	Effects of the Mirror Tilt Angle on the Growth of LiCoO2 Single Crystals by the Traveling Solvent Floating Zone (TSFZ) Technique Using a Tilting-Mirror-type Image Furnace. *Crystal Growth and Design*, **2020**, 20, 3413-3416	3.5	1
397	Application of machine learning potentials to predict grain boundary properties in fcc elemental metals. *Physical Review Materials*, **2020**, 4,	3.2	11
396	Enumeration of nonequivalent substitutional structures using advanced data structure of binary decision diagram. *Journal of Chemical Physics*, **2020**, 153, 104109	3.9	0

395	First-Principles Study on the Stability of Weberite-Type, Pyrochlore, and Defect-Fluorite Structures of A23+B24+O7 (A = Lu3+□a3+, B = Zr4+, Hf4+, Sn4+, and Ti4+). *Journal of Physical Chemistry C*, **2020**, 124, 20555-20562	3.8	3
394	Growth and anisotropy evaluation of NbBiCh3 (Ch = S, Se) misfit-layered superconducting single crystals. *Solid State Communications*, **2020**, 321, 114051	1.6	2
393	Growth and characterization of (La,Ce)OBiS2 single crystals. *Japanese Journal of Applied Physics*, **2019**, 58, 063001	1.4	2
392	Growth of Superconducting Sm(O,F)BiS2 Single Crystals. *Crystal Growth and Design*, **2019**, 19, 6136-6140	3.5	3
391	Crystal Growth and Characterization of LixLa(1□)/3NbO3 by the Traveling Solvent Floating Zone Method. *Crystal Growth and Design*, **2019**, 19, 6291-6295	3.5	4
390	Bulk superconductivity in a four-layer-type Bi-based compound LaOBiAgSnSSe. *Scientific Reports*, **2019**, 9, 13346	4.9	5
389	Self-Combustion Synthesis of Novel Metastable Ternary Molybdenum Nitrides **2019**, 1, 64-70		11
388	Growth and transport properties under high pressure of PrOBiS2 single crystals. *Solid State Communications*, **2019**, 296, 17-20	1.6	3
387	Group-theoretical high-order rotational invariants for structural representations: Application to linearized machine learning interatomic potential. *Physical Review B*, **2019**, 99,	3.3	19
386	A-site cation size effect on oxygen octahedral rotations in acentric Ruddlesden-Popper alkali rare-earth titanates. *Physical Review Materials*, **2019**, 3,	3.2	6
385	Impact of interstitial C on phase stability and stacking-fault energy of the CrMnFeCoNi high-entropy alloy. *Physical Review Materials*, **2019**, 3,	3.2	21
384	Vibrational Effects in X-ray Absorption Spectra of Two-Dimensional Layered Materials. *Journal of Physical Chemistry C*, **2019**, 123, 9688-9692	3.8	5
383	Pressure-induced insulator to metal transition of mixed valence compound Ce(O,F)SbS2. *Journal of Applied Physics*, **2019**, 125, 075102	2.5	6
382	Solution effect on improved structural compatibility of NiTi-based alloys by systematic first-principles calculations. *Journal of Applied Physics*, **2019**, 125, 055106	2.5	2
381	Recommender System of Successful Processing Conditions for New Compounds Based on a Parallel Experimental Data Set. *Chemistry of Materials*, **2019**, 31, 9984-9992	9.6	4
380	Growth of LiCoO2 Single Crystals by the TSFZ Method. *Crystal Growth and Design*, **2019**, 19, 415-420	3.5	4
379	Growth and physical properties of Ce(O,F)Sb(S,Se)2 single crystals with site-selected chalcogen atoms. *Solid State Communications*, **2019**, 289, 38-42	1.6	4
378	Determination of the phase relation of a LixLa(1□)/3NbO3 system by the slow cooling floating zone method. *Journal of Crystal Growth*, **2019**, 507, 251-254	1.6	3

377	Design and synthesis of a magnesium alloy for room temperature hydrogen storage. *Acta Materialia*, **2018**, 149, 88-96	8.4	101
376	Crystal Structure and Superconductivity of Tetragonal and Monoclinic CePr OBiS. *Inorganic Chemistry*, **2018**, 57, 5364-5370	5.1	9
375	First-principles study in an inter-granular glassy film model of silicon nitride. *Journal of the American Ceramic Society*, **2018**, 101, 2673-2688	3.8	11
374	Position effects of mirror□amp system on the growth of rutile crystal based on the infrared convergent-heating floating zone method. *Journal of Crystal Growth*, **2018**, 496-497, 69-73	1.6	1
373	Compositional descriptor-based recommender system for the materials discovery. *Journal of Chemical Physics*, **2018**, 148, 241719	3.9	22
372	Synthesis, crystal structure and optical absorption of NaInS2-Se. *Journal of Alloys and Compounds*, **2018**, 750, 409-413	5.7	5
371	Temperature-dependent phonon spectra of magnetic random solid solutions. *Npj Computational Materials*, **2018**, 4,	10.9	13
370	Lattice thermal conductivities of two SiO2 polymorphs by first-principles calculations and the phonon Boltzmann transport equation. *Physical Review B*, **2018**, 97,	3.3	38
369	Double thermoelectric power factor of a 2D electron system. *Nature Communications*, **2018**, 9, 2224	17.4	35
368	Matrix- and tensor-based recommender systems for the discovery of currently unknown inorganic compounds. *Physical Review Materials*, **2018**, 2,	3.2	29
367	Effects of composition, crystal structure, and surface orientation on band alignment of divalent metal oxides: A first-principles study. *Physical Review Materials*, **2018**, 2,	3.2	16
366	Crystal growth of La Li TiO by the TSFZ method. *Royal Society Open Science*, **2018**, 5, 181445	3.3	4
365	High Rate Performance of Dual-Substituted LiFePO4 Based on Controlling Metastable Intermediate Phase. *ACS Applied Energy Materials*, **2018**, 1, 6736-6740	6.1	5
364	Synthesis of Bi2(O,F)S2 superconductors by NaF treatment. *Journal of the Ceramic Society of Japan*, **2018**, 126, 591-593	1	2
363	Data-centric science for materials innovation. *MRS Bulletin*, **2018**, 43, 659-663	3.2	17
362	Impact of Chemical Fluctuations on Stacking Fault Energies of CrCoNi and CrMnFeCoNi High Entropy Alloys from First Principles. *Entropy*, **2018**, 20,	2.8	42
361	Linearized machine-learning interatomic potentials for non-magnetic elemental metals: Limitation of pairwise descriptors and trend of predictive power. *Journal of Chemical Physics*, **2018**, 148, 234106	3.9	17
360	Thermoelectric phase diagram of the SrTiO3□rNbO3 solid solution system. *Journal of Applied Physics*, **2017**, 121, 185102	2.5	15

359	Theoretical investigation of solid solution states of Ti1−VxH2. *Acta Materialia*, **2017**, 134, 274-282	8.4	2
358	Growth and superconducting properties of Cd-doped La(O,F)BiS2 single crystals. *Solid State Communications*, **2017**, 261, 32-36	1.6	1
357	First-Principles Selection of Solute Elements for Er-Stabilized Bi2O3 Oxide-Ion Conductor with Improved Long-Term Stability at Moderate Temperatures. *Chemistry of Materials*, **2017**, 29, 3763-3768	9.6	20
356	Mode decomposition based on crystallographic symmetry in the band-unfolding method. *Physical Review B*, **2017**, 95,	3.3	23
355	Competing Structural Instabilities in the Ruddlesden−Popper Derivatives HRTiO4 (R = Rare Earths): Oxygen Octahedral Rotations Inducing Noncentrosymmetricity and Layer Sliding Retaining Centrosymmetricity. *Chemistry of Materials*, **2017**, 29, 656-665	9.6	19
354	Band structure diagram paths based on crystallography. *Computational Materials Science*, **2017**, 128, 140-184	3.2	247
353	Thermodynamics of Meissner effect and flux pinning behavior in the bulk of single-crystal La2−SrxCuO4 (x=0.09). *Physical Review B*, **2017**, 96,	3.3	6
352	Direct evidence of hidden local spin polarization in a centrosymmetric superconductor LaO FBiS. *Nature Communications*, **2017**, 8, 1919	17.4	29
351	Materials Design Using First-Principles Calculations for Lithium-Ion Batteries. *Materia Japan*, **2017**, 56, 430-433	0.1	
350	DynaPhoPy: A code for extracting phonon quasiparticles from molecular dynamics simulations. *Computer Physics Communications*, **2017**, 221, 221-234	4.2	48
349	Comparison of approximations in density functional theory calculations: Energetics and structure of binary oxides. *Physical Review B*, **2017**, 96,	3.3	58
348	Synthesis of LaO0.5F0.5BiS2 nanosheets by ultrasonification. *Journal of Asian Ceramic Societies*, **2017**, 5, 183-185	2.4	2
347	Representation of compounds for machine-learning prediction of physical properties. *Physical Review B*, **2017**, 95,	3.3	158
346	Superconductivity and its enhancement under high pressure in F-free single crystals of CeOBiS2. *Journal of Alloys and Compounds*, **2017**, 722, 467-473	5.7	17
345	Unconventional Superconductivity in the BiS_{2}-Based Layered Superconductor NdO_{0.71}F_{0.29}BiS_{2}. *Physical Review Letters*, **2017**, 118, 167002	7.4	44
344	Manifestation of hopping conductivity and granularity within phase diagrams of LaO F BiS, Sr La FBiS and related BiS-based compounds. *Journal of Physics Condensed Matter*, **2017**, 29, 355702	1.8	1
343	Atomistic Origin of Phase Stability in Oxygen-Functionalized MXene: A Comparative Study. *Journal of Physical Chemistry C*, **2017**, 121, 18947-18953	3.8	34
342	Ce 4f electronic states of CeO1−FxBiS2 studied by soft x-ray photoemission spectroscopy. *Physical Review B*, **2017**, 95,	3.3	5

341	First-principles screening of structural properties of intermetallic compounds on martensitic transformation. *Npj Computational Materials*, **2017**, 3,	10.9	9
340	Ultra-severe plastic deformation: Evolution of microstructure, phase transformation and hardness in immiscible magnesium-based systems. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2017**, 701, 158-166	5.3	45
339	Coexistence of superconductivity and charge-density wave in the quasi-one-dimensional material HfTe. *Scientific Reports*, **2017**, 7, 45217	4.9	27
338	Band alignment of semiconductors and insulators using dielectric-dependent hybrid functionals: Toward high-throughput evaluation. *Physical Review B*, **2017**, 95,	3.3	45
337	Control of the solid-liquid interface during growth of a Ce-doped Gd2Si2O7 crystal by the traveling solvent floating zone method. *Journal of Crystal Growth*, **2017**, 468, 465-468	1.6	0
336	Discovery of a Novel Sn(II)-Based Oxide SnMoO for Daylight-Driven Photocatalysis. *Advanced Science*, **2017**, 4, 1600246	13.6	18
335	Effects of growth parameters on silicon molten zone formed by infrared convergent-heating floating zone method. *Journal of Crystal Growth*, **2017**, 459, 105-111	1.6	2
334	New Approaches to Computational Materials Science Using First Principles Methods. *Materia Japan* , **2017**, 56, 234-237	0.1	
333	Conceptual and practical bases for the high accuracy of machine learning interatomic potentials: Application to elemental titanium. *Physical Review Materials*, **2017**, 1,	3.2	35
332	Effects of tilt angle of mirror lamp system on shape of solid liquid interface of silicon melt during floating zone growth using infrared convergent heating. *Journal of Crystal Growth*, **2016**, 433, 24-30	1.6	7
331	Crystal growth and anisotropy of high temperature thermoelectric properties of yttrium borosilicide single crystals. *Journal of Solid State Chemistry*, **2016**, 233, 1-7	3.3	15
330	Low phonon conductivity of layered BiCuOS, BiCuOSe, and BiCuOTe from first principles. *Physical Review B*, **2016**, 94,	3.3	17
329	Stability of the structure of transition elements. *Physical Review B*, **2016**, 93,	3.3	15
328	Prediction model of band gap for inorganic compounds by combination of density functional theory calculations and machine learning techniques. *Physical Review B*, **2016**, 93,	3.3	178
327	Comparative ARPES studies of LaOxF1 BiS2(x = 0.23 and 0.46). *Journal of Physics: Conference Series*, **2016**, 683, 012002	0.3	3
326	Discovery of earth-abundant nitride semiconductors by computational screening and high-pressure synthesis. *Nature Communications*, **2016**, 7, 11962	17.4	133
325	Correction to Structure, Superconductivity, and Magnetism of Ce(O,F)BiS2 Single Crystals. *Crystal Growth and Design*, **2016**, 16, 2459-2459	3.5	
324	Categorization of surface polarity from a crystallographic approach. *Computational Materials Science*, **2016**, 113, 221-230	3.2	31

323	structure in steel: A first-principles study. *Journal of Alloys and Compounds*, **2016**, 684, 624-627	5.7	16
322	Pure H? conduction in oxyhydrides. *Science*, **2016**, 351, 1314-7	33.3	110
321	New nanostructured phases with reversible hydrogen storage capability in immiscible magnesium irconium system produced by high-pressure torsion. *Acta Materialia*, **2016**, 108, 293-303	8.4	54
320	Toward Materials Discovery with First-Principles Datasets and Learning Methods. *Springer Series in Materials Science*, **2016**, 173-186	0.9	
319	Impacts of first principles calculations in engineering ceramics. *Journal of the Ceramic Society of Japan*, **2016**, 124, 791-795	1	3
318	First-principles calculations of high-pressure phase transition of TiO2 during decompression: From baddeleyite-type TiO2 to -PbO2-type TiO2. *Journal of Applied Physics*, **2016**, 120, 142108	2.5	2
317	Floating Zone Growth and Characterization of (Ca Nd)AlO (~ 0.001) Single Crystals. *ACS Omega*, **2016**, 1, 1157-1163	3.9	4
316	Suppression of lattice thermal conductivity by mass-conserving cation mutation in multi-component semiconductors. *APL Materials*, **2016**, 4, 104809	5.7	8
315	Improper Inversion Symmetry Breaking and Piezoelectricity through Oxygen Octahedral Rotations in Layered Perovskite Family, LiRTiO4 (R = Rare Earths). *Advanced Electronic Materials*, **2016**, 2, 1500196	6.4	25
314	Growth and Structure of Ce(O,F)SbS2 Single Crystals. *Crystal Growth and Design*, **2016**, 16, 3037-3042	3.5	17
313	Electronic Structure and Defect Chemistry of Tin(II) Complex Oxide SnNb2O6. *Journal of Physical Chemistry C*, **2016**, 120, 9604-9611	3.8	19
312	Conventional s-Wave Superconductivity in BiS2-Based NdO0.71F0.29BiS2 Revealed by Thermal Transport Measurements. *Journal of the Physical Society of Japan*, **2016**, 85, 073707	1.5	29
311	Bulk sensitive angle-resolved photoelectron spectroscopy on Nd(O,F)BiS2. *Journal of Physics: Conference Series*, **2016**, 683, 012003	0.3	2
310	Superconductivity in CeOBiS2 with cerium valence fluctuation. *Solid State Communications*, **2016**, 245, 11-14	1.6	23
309	First-principles calculations of oxygen vacancy formation and metallic behavior at a MnO2 grain boundary. *ACS Applied Materials & Interfaces*, **2015**, 7, 1726-34	9.5	38
308	Crystal structure, defect chemistry and oxygen ion transport of the ferroelectric perovskite, Na0.5Bi0.5TiO3: insights from first-principles calculations. *Journal of Materials Chemistry A*, **2015**, 3, 16574-16582	7.3	63
307	Distributions of phonon lifetimes in Brillouin zones. *Physical Review B*, **2015**, 91,	3.3	607
306	Li Intercalation into a MnO2 Grain Boundary. *ACS Applied Materials & Interfaces*, **2015**, 7, 8125-31	9.5	14

305	Special quasirandom structure in heterovalent ionic systems. *Physical Review B*, **2015**, 91,	3.3	5
304	YB48 the metal rich boundary of YB66; crystal growth and thermoelectric properties. *Journal of Physics and Chemistry of Solids*, **2015**, 87, 221-227	3.9	16
303	C-axis electrical resistivity of PrO1−xFaBiS2single crystals. *Japanese Journal of Applied Physics*, **2015**, 54, 083101	1.4	20
302	First principles phonon calculations in materials science. *Scripta Materialia*, **2015**, 108, 1-5	5.6	4076
301	Structure, Superconductivity, and Magnetism of Ce(O,F)BiS2 Single Crystals. *Crystal Growth and Design*, **2015**, 15, 39-44	3.5	29
300	Growth of Cu(In,Ga)S 2 single crystals using CsCl flux. *Journal of Crystal Growth*, **2015**, 412, 16-19	1.6	2
299	First-principles interatomic potentials for ten elemental metals via compressed sensing. *Physical Review B*, **2015**, 92,	3.3	52
298	Prediction of Low-Thermal-Conductivity Compounds with First-Principles Anharmonic Lattice-Dynamics Calculations and Bayesian Optimization. *Physical Review Letters*, **2015**, 115, 205901	7.4	275
297	Stability of 12CaO·7Al2O3 Crystal under High-Pressure: Experimental and First-Principles Approaches. *Materials Transactions*, **2015**, 56, 1350-1353	1.3	3
296	Influence of the exchange-correlation functional on the quasi-harmonic lattice dynamics of II-VI semiconductors. *Journal of Chemical Physics*, **2015**, 143, 064710	3.9	60
295	Selective fabrication of n- and p-type SnO films without doping. *Physica Status Solidi - Rapid Research Letters*, **2015**, 9, 192-196	2.5	16
294	Proton trapping in Y and Sn Co-doped BaZrO3. *Journal of Materials Chemistry A*, **2015**, 3, 10045-10051	13	24
293	Axis symmetry of silicon molten zone interface shape under a mirror-shifting-type infrared convergent-heating floating-zone method. *CrystEngComm*, **2015**, 17, 9452-9458	3.3	3
292	Epitaxial growth of tin(II) niobate with a pyrochlore structure. *Journal of Crystal Growth*, **2015**, 416, 126-129	1.6	4
291	First-Principles Insight into the Hydration Ability and Proton Conduction of the Solid State Proton Conductor, Y and Sn Co-Doped BaZrO3. *Chemistry of Materials*, **2015**, 27, 901-908	9.6	56
290	Superconducting double perovskite bismuth oxide prepared by a low-temperature hydrothermal reaction. *Angewandte Chemie - International Edition*, **2014**, 53, 3599-603	16.4	48
289	Impact of local strain on Ti-L□electron energy-loss near-edge structures of BaTiO□a first-principles multiplet study. *Microscopy (Oxford, England)*, **2014**, 63, 249-54	1.3	9
288	Inversion symmetry breaking by oxygen octahedral rotations in the Ruddlesden-Popper NaRTiO4 family. *Physical Review Letters*, **2014**, 112, 187602	7.4	45

287	Zr coordination change during crystallization of MgOAl2O3SiO2ZrO2 glass ceramics. *Journal of Non-Crystalline Solids*, **2014**, 384, 47-54	3.9	28
286	Photocatalytic activity of -PbO2-type TiO2. *Physica Status Solidi - Rapid Research Letters*, **2014**, 8, 822-826	2.5	12
285	Local Structure and Energetics of Pr- and La-Doped SrTiO3 Grain Boundaries and the Influence on CoreShell Structure Formation. *Journal of Physical Chemistry C*, **2014**, 118, 25765-25778	3.8	17
284	Efficient determination of alloy ground-state structures. *Physical Review B*, **2014**, 90,	3.3	9
283	Oxygen vacancy formation and reduction properties of MnO2 grain boundaries and the potential for high electrochemical performance. *ACS Applied Materials & Interfaces*, **2014**, 6, 17776-84	9.5	36
282	Effects of lamp power and mirror position on the interface shape of the silicon molten zone during infrared convergent heating. *CrystEngComm*, **2014**, 16, 4619-4623	3.3	11
281	First principles study of dopant solubility and defect chemistry in LiCoO2. *Journal of Materials Chemistry A*, **2014**, 2, 11235-11245	13	46
280	Phonon softening in paramagnetic bcc Fe and its relationship to the pressure-induced phase transition. *Physical Review B*, **2014**, 90,	3.3	29
279	Proton incorporation and trapping in ZrO2 grain boundaries. *Journal of Materials Chemistry A*, **2014**, 2, 1400-1408	13	17
278	Accelerated discovery of cathode materials with prolonged cycle life for lithium-ion battery. *Nature Communications*, **2014**, 5, 4553	17.4	86
277	Feed Size Dependence of Position Effects of Mirror-Lamp System on Shape of Silicon Crystal during Its Growth by Mirror-Shifting-Type Infrared Convergent-Heating Floating Zone Method. *Crystal Growth and Design*, **2014**, 14, 5117-5121	3.5	6
276	Significant reduction in hydration energy for yttria stabilized zirconia grain boundaries and the consequences for proton conduction. *Langmuir*, **2014**, 30, 10456-64	4	8
275	Surface design of alloy protection against CO-poisoning from first principles. *Journal of Physics Condensed Matter*, **2014**, 26, 355006	1.8	2
274	Protonic defects in yttria stabilized zirconia: incorporation, trapping and migration. *Physical Chemistry Chemical Physics*, **2014**, 16, 4814-22	3.6	13
273	Cytotoxicity of stoichiometric hydroxyapatites with different crystallite sizesPeer review under responsibility of The Ceramic Society of Japan and the Korean Ceramic Society.View all notes. *Journal of Asian Ceramic Societies*, **2014**, 2, 64-67	2.4	7
272	Crystal structures of LaO1FxBiS2 (x~0.23, 0.46): Effect of F doping on distortion of BiS plane. *Journal of Solid State Chemistry*, **2014**, 212, 213-217	3.3	55
271	Growth and superconducting properties of F-substituted ROBiS2 (R=La, Ce, Nd) single crystals. *Solid State Communications*, **2014**, 178, 33-36	1.6	73
270	Thermal physics of the lead chalcogenides PbS, PbSe, and PbTe from first principles. *Physical Review B*, **2014**, 89,	3.3	172

269	Atomic structure of luminescent centers in high-efficiency Ce-doped w-AlN single crystal. *Scientific Reports*, **2014**, 4, 3778	4.9	34
268	Superconducting Anisotropies of F-Substituted LaOBiSe2 Single Crystals. *Journal of the Physical Society of Japan*, **2014**, 83, 114709	1.5	22
267	Proximity to Fermi-surface topological change in superconducting LaO0.54F0.46BiS2. *Physical Review B*, **2014**, 90,	3.3	31
266	An Improved Method for Quantitatively Predicting the Electrochemical Stabilities of Organic Liquid Electrolytes Using Ab Initio Calculations. *Journal of the Electrochemical Society*, **2014**, 161, G7-G14	3.9	11
265	Mn L2,3-edge X-ray absorption spectroscopic studies on charge-discharge mechanism of Li2MnO3. *Applied Physics Letters*, **2014**, 104, 053906	3.4	37
264	Sparse representation for a potential energy surface. *Physical Review B*, **2014**, 90,	3.3	59
263	Machine learning with systematic density-functional theory calculations: Application to melting temperatures of single- and binary-component solids. *Physical Review B*, **2014**, 89,	3.3	179
262	Cluster expansion of multicomponent ionic systems with controlled accuracy: importance of long-range interactions in heterovalent ionic systems. *Journal of Physics Condensed Matter*, **2014**, 26, 115403	1.8	6
261	High-pressure torsion of titanium at cryogenic and room temperatures: Grain size effect on allotropic phase transformations. *Acta Materialia*, **2014**, 68, 207-213	8.4	62
260	Effect of local coordination of Mn on Mn-L2,3 edge electron energy loss spectrum. *Journal of Applied Physics*, **2013**, 114, 054906	2.5	19
259	Strong Spin-Lattice Coupling Through Oxygen Octahedral Rotation in Divalent Europium Perovskites. *Advanced Functional Materials*, **2013**, 23, 1864-1872	15.6	28
258	Ground state of the singly ionized oxygen vacancy in rutile TiO2. *Journal of Applied Physics*, **2013**, 114, 113702	2.5	20
257	First-principles study of valence band offsets at ZnSnP2/CdS, ZnSnP2/ZnS, and related chalcopyrite/zincblende heterointerfaces. *Journal of Applied Physics*, **2013**, 114, 043718	2.5	18
256	Functional complex point-defect structure in a huge-size-mismatch system. *Physical Review Letters*, **2013**, 110, 065504	7.4	33
255	Anti-ferrodistortive-like oxygen-octahedron rotation induced by the oxygen vacancy in cubic SrTiO3. *Advanced Materials*, **2013**, 25, 86-90	24	76
254	Variation of Zr-L2,3 XANES in tetravalent zirconium oxides. *Journal of Physics Condensed Matter*, **2013**, 25, 165505	1.8	15
253	High temperature defect chemistry in layered lithium transition-metal oxides based on first-principles calculations. *Journal of Power Sources*, **2013**, 244, 592-596	8.9	16
252	Accelerated Materials Design of Lithium Superionic Conductors Based on First-Principles Calculations and Machine Learning Algorithms. *Advanced Energy Materials*, **2013**, 3, 980-985	21.8	139

251	Evolution of crystal structures in metallic elements. *Physical Review B*, **2013**, 87,	3.3	56
250	Valence band offsets at zinc-blende heterointerfaces with misfit dislocations: A first-principles study. *Physical Review B*, **2013**, 88,	3.3	10
249	Structural Analysis and Superconducting Properties of F-Substituted NdOBiS2 Single Crystals. *Journal of the Physical Society of Japan*, **2013**, 82, 113701	1.5	83
248	Band offsets of CuInSe2/CdS and CuInSe2/ZnS (110) interfaces: A hybrid density functional theory study. *Physical Review B*, **2013**, 88,	3.3	38
247	Theoretical Photovoltaic Conversion Efficiencies of ZnSnP2, CdSnP2, and Zn1-xCdxSnP2Alloys. *Applied Physics Express*, **2013**, 6, 061201	2.4	31
246	Vanadium L2,3 XANES experiments and first-principles multielectron calculations: Impact of second-nearest neighboring cations on vanadium-bearing fresnoites. *American Mineralogist*, **2013**, 98, 665-670	2.9	5
245	Local environment of silicon in cubic boron nitride. *Journal of Applied Physics*, **2013**, 114, 233502	2.5	10
244	Theoretical Calculations of Segregation Behavior of Zinc and Magnesium at Hydroxyapatite Surface in Contact with Water. *Materials Transactions*, **2013**, 54, 1262-1267	1.3	2
243	Growth of large La2−xSrxCuO4 single crystals using tilting-mirror-type infrared heating image furnace. *Physica C: Superconductivity and Its Applications*, **2012**, 472, 87-91	1.3	5
242	Atomic-level modeling and computation of intergranular glassy film in high-purity Si3N4 ceramics. *Journal of the European Ceramic Society*, **2012**, 32, 1301-1311	6	6
241	Crystal and electronic structure and magnetic properties of divalent europium perovskite oxides EuMO3 (M = Ti, Zr, and Hf): experimental and first-principles approaches. *Inorganic Chemistry*, **2012**, 51, 4560-7	5.1	38
240	Ionization potentials of (112) and (112̄) facet surfaces of CuInSe2 and CuGaSe2. *Physical Review B*, **2012**, 86,	3.3	59
239	Nitrogen and hydrogen defect equilibria in Ca12Al14O33: a combined experimental and computational study. *Journal of Materials Chemistry*, **2012**, 22, 15828		13
238	Inducement of Superconductivity in Fe(Te,S) by Sulfuric Acid Treatment. *Journal of the Physical Society of Japan*, **2012**, 81, 085005	1.5	5
237	Defect chemistry of a BaZrO3 Σ3 (111) grain boundary by first principles calculations and space-charge theory. *Physical Chemistry Chemical Physics*, **2012**, 14, 12339-46	3.6	44
236	Proton-Conducting Network in Lanthanum Orthophosphate. *Journal of Physical Chemistry C*, **2012**, 116, 19117-19124	3.8	38
235	Defect Chemistry in Layered LiMO2 (M = Co, Ni, Mn, and Li1/3Mn2/3) by First-Principles Calculations. *Chemistry of Materials*, **2012**, 24, 3886-3894	9.6	110
234	Crystal growth of rutile by tilting-mirror-type floating zone method. *Journal of Crystal Growth*, **2012** , 360, 105-110	1.6	13

233	Growth of Ba3In4Cu3O12 single-crystal whiskers. *Journal of Crystal Growth*, **2012**, 346, 61-63	1.6	
232	First-Principles Study on Relaxor-Type Ferroelectric Behavior without Chemical Inhomogeneity in BaTaO2N and SrTaO2N. *Chemistry of Materials*, **2012**, 24, 4343-4349	9.6	61
231	Ground-state search in multicomponent magnetic systems. *Physical Review B*, **2012**, 85,	3.3	3
230	Macroscopic quantum tunneling and phase diffusion in a La2−xSrxCuO4 intrinsic Josephson junction stack. *Physical Review B*, **2012**, 86,	3.3	9
229	Tetravalent dysprosium in a perovskite-type oxide. *Advanced Materials*, **2012**, 24, 2051-3	24	20
228	Cluster expansion with controlled accuracy for the MgO/ZnO pseudobinary system via first-principles calculations. *Physical Review B*, **2012**, 86,	3.3	9
227	Site preference of cation vacancies in Mn-doped Ga2O3 with defective spinel structure. *Applied Physics Letters*, **2012**, 101, 241906	3.4	8
226	First-principles molecular dynamics study for average structure and oxygen diffusivity at high temperature in cubic Bi2O3. *Journal of Physics Condensed Matter*, **2012**, 24, 475402	1.8	12
225	Point defects in ZnO: an approach from first principles. *Science and Technology of Advanced Materials*, **2011**, 12, 034302	7.1	234
224	Atomic and electronic structures of the SrVO3-LaAlO3 interface. *Journal of Applied Physics*, **2011**, 110, 046104	2.5	14
223	First-principles thermodynamics of La2O3-P2O5 pseudobinary system. *Physical Review B*, **2011**, 84,	3.3	14
222	Atomistic structure and energetics of interface between Mn-doped β-Ga2O3 and MgAl2O4. *Journal of Materials Science*, **2011**, 46, 4169-4175	4.3	9
221	Antiferromagnetic superexchange via 3d states of titanium in EuTiO3 as seen from hybrid Hartree-Fock density functional calculations. *Physical Review B*, **2011**, 83,	3.3	86
220	Theoretical Fingerprints of Transition Metal L2,3 XANES and ELNES for Lithium Transition Metal Oxides by ab Initio Multiplet Calculations. *Journal of Physical Chemistry C*, **2011**, 115, 11871-11879	3.8	32
219	Electronic and structural properties of the oxygen vacancy in BaTiO3. *Applied Physics Letters*, **2011**, 98, 172901	3.4	49
218	Effects of the diameter of rutile (TiO2) single crystals grown using tilting-mirror-type infrared heating image furnace on solid–liquid interface and etch pit density. *Journal of Crystal Growth*, **2011**, 317, 135-138	1.6	14
217	Electronic structures of dynamically stable As2O3, Sb2O3, and Bi2O3 crystal polymorphs. *Physical Review B*, **2011**, 83,	3.3	33
216	Synthesis and electrochemistry of monoclinic Li(MnxFe1−x)BO3: a combined experimental and computational study. *Journal of Materials Chemistry*, **2011**, 21, 10690		45

215	Phonon-phonon interactions in transition metals. *Physical Review B*, **2011**, 84,	3.3	235
214	Ab initio charge transfer multiplet calculations on the L2,3 XANES and ELNES of 3d transition metal oxides. *Physical Review B*, **2011**, 83,	3.3	88
213	Fabrication of submicron La2−xSrxCuO4 intrinsic Josephson junction stacks. *Journal of Applied Physics*, **2011**, 109, 033912	2.5	5
212	Epitaxial growth of Mn-doped β-Ga2O3 on spinel substrate. *Journal of Materials Research*, **2011**, 26, 578-583	2.5	35
211	First-Principles Calculations of Phase Transition in CaTiO3 under Negative Static Pressure. *Journal of the Korean Physical Society*, **2011**, 59, 2497-2502	0.6	5
210	First-principles phonon calculations of thermal expansion in Ti3SiC2, Ti3AlC2, and Ti3GeC2. *Physical Review B*, **2010**, 81,	3.3	309
209	Anisotropic phonon density of states in FePt nanoparticles with L10 structure. *Physical Review B*, **2010**, 81,	3.3	9
208	Theoretical study on the structure and energetics of intergranular glassy film in Si3N4-SiO2 ceramics. *International Journal of Materials Research*, **2010**, 101, 57-65	0.5	7
207	Phase relationships and structures of inorganic crystals by a combination of the cluster expansion method and first principles calculations. *Journal of Physics Condensed Matter*, **2010**, 22, 384207	1.8	1
206	Inter-granular glassy phases in the low-CaO-doped HIPed Si3N4 ceramics: a review. *International Journal of Materials Research*, **2010**, 101, 66-74	0.5	6
205	Growth and Anisotropic Properties of RBa2Cu3OxSingle-Crystal Whiskers. *Japanese Journal of Applied Physics*, **2010**, 49, 033101	1.4	3
204	Classification of spinel structures based on first-principles cluster expansion analysis. *Physical Review B*, **2010**, 81,	3.3	27
203	Reduced Etch Pit Density of Rutile (TiO2) Single Crystals by Growth Using a Tilting-Mirror-Type Infrared Heating Image Furnace. *Crystal Growth and Design*, **2010**, 10, 3929-3930	3.5	8
202	Thermodynamics and structures of oxide crystals by a systematic set of first principles calculations. *Journal of Materials Chemistry*, **2010**, 20, 10335		7
201	Effects of Off-Stoichiometry of LiC6 on the Lithium Diffusion Mechanism and Diffusivity by First Principles Calculations. *Journal of Physical Chemistry C*, **2010**, 114, 2375-2379	3.8	84
200	Structures and energetics of Bi2O3 polymorphs in a defective fluorite family derived by systematic first-principles lattice dynamics calculations. *Physical Review B*, **2010**, 81,	3.3	25
199	Singular ring-shaped distribution of Nd in NdxY1-xVO4 crystals grown by floating zone method. *Crystal Research and Technology*, **2010**, 45, 692-696	1.3	1
198	Lithium iron borates as high-capacity battery electrodes. *Advanced Materials*, **2010**, 22, 3583-7	24	204

197	Effects of tilting mirrors on the solid–liquid interface during floating zone growth using tilting-mirror-type infrared-heating image furnace. *Journal of Crystal Growth*, **2010**, 312, 2008-2011	1.6	18
196	Theoretical ELNES using one-particle and multi-particle calculations. *Micron*, **2010**, 41, 695-709	2.3	72
195	First-principles prediction of low-energy structures for AlH3. *Physical Review B*, **2009**, 79,	3.3	7
194	First-principles study of defect-induced potentials in Ca2CuO2Cl2. *Physical Review B*, **2009**, 80,	3.3	5
193	First-principles calculations of x-ray absorption near edge structure and energy loss near edge structure: present and future. *Journal of Physics Condensed Matter*, **2009**, 21, 104201	1.8	26
192	Lattice dynamics and thermal properties of SrHfO3 by first-principles calculations. *Physica Status Solidi (B): Basic Research*, **2009**, 246, 1628-1633	1.3	9
191	Growth of Nd-doped YVO4 single crystals along <100>tetra by the anisotropic heating floating zone method. *Journal of Crystal Growth*, **2009**, 311, 4535-4537	1.6	3
190	First-principles study on lithium removal from Li2MnO3. *Journal of Power Sources*, **2009**, 189, 798-801	8.9	136
189	27Al NMR Chemical Shifts in Oxide Crystals: A First-Principles Study. *Journal of Physical Chemistry C*, **2009**, 113, 3869-3873	3.8	44
188	First-principles investigation of atomic structures and stability of proton-exchanged layered sodium titanate. *Physical Review B*, **2009**, 79,	3.3	18
187	Cluster expansion method for multicomponent systems based on optimal selection of structures for density-functional theory calculations. *Physical Review B*, **2009**, 80,	3.3	92
186	Beam damage suppression of low-kappa porous Si-O-C films by cryo-electron-energy loss spectroscopy (EELS). *Journal of Electron Microscopy*, **2009**, 58, 29-34		6
185	First Principles Lattice Dynamics Calculations of Ag+ Doped KX (X=Cl, Br and I). *Materials Transactions*, **2009**, 50, 999-1003	1.3	
184	Observation of macroscopic quantum tunneling in La2-xSrxCuO4intrinsic Josephson Junctions. *Journal of Physics: Conference Series*, **2009**, 150, 052132	0.3	1
183	SYNTHESIS AND ELECTRICAL CONDUCTIVITY OF TETRA-VALENT CERIUM POLYPHOSPHATE BULKS. *Phosphorus Research Bulletin*, **2009**, 23, 20-24	0.3	7
182	Geometric ferroelectricity in rare-earth compounds RGaO3 and RInO3. *Physical Review B*, **2009**, 79,	3.3	36
181	First-principles study of native defects and lanthanum impurities in NaTaO3. *Physical Review B*, **2008**, 78,	3.3	52
180	First-principles calculations of the ferroelastic transition between rutile-type and CaCl2-type SiO2 at high pressures. *Physical Review B*, **2008**, 78,	3.3	3593

179	First-principles approach to chemical diffusion of lithium atoms in a graphite intercalation compound. *Physical Review B*, **2008**, 78,	3.3	160
178	Lattice dynamics and thermodynamical properties of silicon nitride polymorphs. *Physical Review B*, **2008**, 78,	3.3	71
177	First principles calculations for modern ceramic science and engineering. *Journal of Physics Condensed Matter*, **2008**, 20, 064215	1.8	4
176	Transition pathway of CO2 crystals under high pressures. *Physical Review B*, **2008**, 77,	3.3	54
175	First-principles-based phase diagram of the cubic BNC ternary system. *Physical Review B*, **2008**, 77,	3.3	33
174	First Principles Calculation of CO and H2 Adsorption on Strained Pt Surface. *Materials Transactions*, **2008**, 49, 2484-2490	1.3	4
173	Influence of lanthanum addition on preparation and powder properties of cobalt phosphates. *Journal of Materials Science*, **2008**, 43, 5483-5488	4.3	19
172	Intrinsic Josephson properties of. *Physica C: Superconductivity and Its Applications*, **2008**, 468, 1922-1924	1.3	4
171	First-principles investigation of R2O3(ZnO)3 (R=Al, Ga, and In) in homologous series of compounds. *Journal of Solid State Chemistry*, **2008**, 181, 137-142	3.3	10
170	Nanoporous crystal 12CaO.7Al2O3: a playground for studies of ultraviolet optical absorption of negative ions. *Journal of Physical Chemistry B*, **2007**, 111, 1946-56	3.4	57
169	INFLUENCE OF UREA ADDITION ON PREPARATION AND ACIDIC PROPERTIES OF AMORPHOUS LANTHANUM PYROPHOSPHATE. *Phosphorus Research Bulletin*, **2007**, 21, 53-59	0.3	1
168	AgB2: Superconductivity and the role of paramagnons. *Physica C: Superconductivity and Its Applications*, **2007**, 466, 76-81	1.3	8
167	Thermal annealing effect on magnetism and cation distribution in disordered ZnFe2O4 thin films deposited on glass substrates. *Journal of Magnetism and Magnetic Materials*, **2007**, 310, 2543-2545	2.8	35
166	Possible experimental signature of charge-orbital density waves in Nd1−xCa1+xMnO4: Heat capacity and magnetization study. *Physical Review B*, **2007**, 75,	3.3	2
165	X-ray absorption near-edge structures of disordered Mg1−xZnxO solid solutions. *Physical Review B*, **2007**, 76,	3.3	15
164	Direct observation of quantized interlayer vortex flow in a high-Tc La1.87Sr0.13CuO4 single crystal. *Applied Physics Letters*, **2007**, 91, 202511	3.4	2
163	First-principles XANES simulations of spinel zinc ferrite with a disordered cation distribution. *Physical Review B*, **2007**, 75,	3.3	88
162	Current-induced in-plane superconducting transition in intrinsic Josephson junctions. *Superconductor Science and Technology*, **2006**, 19, S209-S212	3.1	3

161	Growth and characterization of Ca doped Eu-123 whiskers for intrinsic Josephson junction applications. *Superconductor Science and Technology*, **2006**, 19, 290-293	3.1	3
160	Electron Carrier Generation in a Refractory Oxide 12CaO·7Al2O3 by Heating in Reducing Atmosphere: Conversion from an Insulator to a Persistent Conductor. *Journal of the American Ceramic Society*, **2006**, 89, 3294-3298	3.8	56
159	Growth mechanism of EuBa2Cu3Ox single-crystalline whiskers from Ca and Te doped precursors. *Journal of Crystal Growth*, **2006**, 289, 192-196	1.6	4
158	Ab initio lattice dynamics and phase transformations of ZrO2. *Physical Review B*, **2005**, 71,	3.3	90
157	Transport characteristics in c-axis La/sub 2-x/Sr/sub x/CuO/sub 4/ (LSCO) single crystals. *IEEE Transactions on Applied Superconductivity*, **2005**, 15, 3782-3785	1.8	5
156	Electronic structure and x-ray-absorption near-edge structure of amorphous Zr-oxide and Hf-oxide thin films: A first-principles study. *Journal of Applied Physics*, **2005**, 97, 073519	2.5	6
155	Local Geometry and Energetics of Hydrogen in Orthorhombic SrZrO3. *Materials Transactions*, **2005**, 46, 1106-1111	1.3	13
154	Electronic Structures of Ln3+-SiAlONs with Correlations to Solubility and Solution Effects. *Journal of the American Ceramic Society*, **2005**, 79, 2527-2532	3.8	19
153	Local Chemical Bonding around Rare-Earth Ions in - and Si3N4. *Journal of the American Ceramic Society*, **2005**, 80, 2525-2532	3.8	22
152	Calculation of Grain-Boundary Bonding in Rare-Earth-Doped Si3N4. *Journal of the American Ceramic Society*, **2005**, 81, 565-570	3.8	21
151	XANES and ELNES in Ceramic Science. *Journal of the American Ceramic Society*, **2005**, 88, 2013-2029	3.8	104
150	Behavior of oxygen bubbles during crystal growth of Ca12Al14O33 by floating method in magnetic field. *Crystal Research and Technology*, **2005**, 40, 329-333	1.3	10
149	Prediction of the X-ray absorption near edge structure of the new high-density phase of SiO2. *Physica Status Solidi (B): Basic Research*, **2005**, 242, R94-R96	1.3	8
148	Growth and superconducting properties of (Eu,R)Ba2Cu3O7 (R = Er, Tm) single-crystalline whiskers. *Superconductor Science and Technology*, **2005**, 18, 1238-1243	3.1	3
147	Infrared furnace with a superconducting magnet for floating zone growth of oxide single crystals. *Review of Scientific Instruments*, **2005**, 76, 035104	1.7	3
146	Decomposition reactions for NaAlH4, Na3AlH6, and NaH: First-principles study. *Physical Review B*, **2005**, 71,	3.3	93
145	Electronic insulator-conductor conversion in hydride ion-doped 12CaO·7Al2O3 by electron-beam irradiation. *Applied Physics Letters*, **2005**, 86, 022109	3.4	21
144	Cubic and orthorhombic structures of aluminum hydride AlH3 predicted by a first-principles study. *Physical Review B*, **2005**, 71,	3.3	65

143	Distribution of solute atoms in □and spinel Si6□AlzOzN8□ by Al K-edge x-ray absorption near-edge structure. *Physical Review B*, **2005**, 71,	3.3	37
142	Core-hole effect on dipolar and quadrupolar transitions of SrTiO3 and BaTiO3 at Ti K edge. *Physical Review B*, **2005**, 71,	3.3	46
141	Differential Conductance Properties of La2-xSrxCuO4Intrinsic Josephson Junctions under Magnetic Field. *Japanese Journal of Applied Physics*, **2004**, 43, 124-125	1.4	0
140	Suppression of the superconducting energy gap in intrinsic Josephson junctions of Bi2Sr2CaCu2O8+□single crystals. *Superconductor Science and Technology*, **2004**, 17, 1160-1164	3.1	10
139	First-principles calculations of ELNES and XANES of selected wide-gap materials: Dependence on crystal structure and orientation. *Physical Review B*, **2004**, 70,	3.3	148
138	Theoretical Prediction of Post-Spinel Phases of Silicon Nitride. *Journal of the American Ceramic Society*, **2004**, 85, 7-10	3.8	23
137	Solubility of Si3N4 in Liquid SiO2. *Journal of the American Ceramic Society*, **2004**, 85, 25-32	3.8	33
136	First-Principles Calculations of Anion Vacancies in Oxides and Nitrides. *Journal of the American Ceramic Society*, **2004**, 85, 68-74	3.8	47
135	Theoretical Prediction of the Structure and Properties of Cubic Spinel Nitrides. *Journal of the American Ceramic Society*, **2004**, 85, 75-80	3.8	86
134	Effective Doping in Cubic Si3N4 and Ge3N4: A First-Principles Study. *Journal of the American Ceramic Society*, **2004**, 85, 97-100	3.8	31
133	Theoretical Study on the Chemistry of Intergranular Glassy Film in Si3N4□iO2 Ceramics. *Journal of the American Ceramic Society*, **2004**, 85, 109-112	3.8	36
132	Characteristics of rutile single crystals grown under two different oxygen partial pressures. *Journal of Crystal Growth*, **2004**, 268, 103-107	1.6	9
131	Reduced SnO2 surfaces by first-principles calculations. *Applied Physics Letters*, **2004**, 84, 909-911	3.4	85
130	Atomistic mechanism of proton conduction in solid CsHSO4 by a first-principles study. *Physical Review B*, **2004**, 69,	3.3	22
129	Valence state of Ti in conductive nanowires in sapphire. *Physical Review B*, **2004**, 70,	3.3	22
128	Superoxide Ion Encaged in Nanoporous Crystal 12CaO□7Al2O3 Studied by Continuous Wave and Pulsed Electron Paramagnetic Resonance. *Journal of Physical Chemistry B*, **2004**, 108, 18557-18568	3.4	37
127	Free-Energy Calculation of Precipitate Nucleation in an Fe-Cu-Ni Alloy. *Materials Transactions*, **2004**, 45, 1978-1981	1.3	28
126	First-principles Calculation of L3 X-ray Absorption Near Edge Structures (XANES) and Electron Energy Loss Near Edge Structures (ELNES) of GaN and InN Polymorphs. *Materials Transactions*, **2004**, 45, 2023-2025	1.3	5

125	Theoretical Investigation of Al K-edge X-ray Absorption Spectra of Al, AlN and Al2O3. *Materials Transactions*, **2004**, 45, 2031-2034	1.3	18
124	Electronic States of Sulfur Doped TiO2 by First Principles Calculations. *Materials Transactions*, **2004**, 45, 1987-1990	1.3	35
123	First Principles Study of Core-hole Effect on Fluorine K-edge X-ray Absorption Spectra of MgF2 and ZnF2. *Materials Transactions*, **2004**, 45, 1991-1993	1.3	6
122	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
121	Energy Level Structure of LiYF4:Dy3+: Crystal Field Analysis. *Materials Transactions*, **2004**, 45, 2026-2030	1.3	8
120	X-ray Absorption Near Edge Structures of Silicon Nitride Thin Film by Pulsed Laser Deposition. *Materials Transactions*, **2004**, 45, 2039-2041	1.3	3
119	Coordination and Interface Analysis of Atomic-Layer-Deposition Al2O3 on Si (001) Using EELS. *Materia Japan*, **2004**, 43, 982-982	0.1	
118	High-Density Electron Anions in a Nanoporous Single Crystal: [Ca24Al28O64]4+(4e-).. *ChemInform*, **2003**, 34, no		1
117	Depression of the superconducting transition temperature in neutron irradiated La2CuO4+□ *Physica C: Superconductivity and Its Applications*, **2003**, 388-389, 369-370	1.3	2
116	Effect of substrates on superconductivity and composition of the IR-LPE La2□SrxCuO4 single crystalline films. *Physica C: Superconductivity and Its Applications*, **2003**, 392-396, 1302-1305	1.3	
115	Identification of ultradilute dopants in ceramics. *Nature Materials*, **2003**, 2, 541-5	27	72
114	High-density electron anions in a nanoporous single crystal: [Ca24Al28O64]4+(4e-). *Science*, **2003**, 301, 626-9	33.3	638
113	Observation of diamagnetic precursor to the Meissner state above Tc in high-Tc La2□SrxCuO4 cuprates by scanning SQUID microscopy. *Physica C: Superconductivity and Its Applications*, **2002**, 367, 9-14	1.3	8
112	Characterization of intrinsic Josephson junctions for La2□SrxCuO4 single crystals. *Physica C: Superconductivity and Its Applications*, **2002**, 367, 382-387	1.3	4
111	Temperature dependent polarized XANES spectra for Zn-doped LSCO system. *Physica C: Superconductivity and Its Applications*, **2002**, 378-381, 78-83	1.3	2
110	The growth of TiO2 (rutile) single crystals using the FZ method under high oxygen pressure. *Journal of Crystal Growth*, **2002**, 237-239, 730-734	1.6	9
109	Crystal growth of Ca12Al14O33 by the floating zone method. *Journal of Crystal Growth*, **2002**, 237-239, 801-805	1.6	71
108	Formation energy of Cr/Al vacancies in spinel MgCr2O4 and MgAl2O4 by first-principles calculations. *Physical Review B*, **2002**, 65,	3.3	19

107	Energetics of Hydrogen States in SrZrO3. *Materials Transactions*, **2002**, 43, 1444-1450	1.3	10
106	Evaluation of Migration Energy of Lithium Ions in Chalcogenides and Halides by First Principles Calculation. *Materials Transactions*, **2002**, 43, 1460-1463	1.3	26
105	Theoretical Formation Energy of Oxygen-Vacancies in Oxides. *Materials Transactions*, **2002**, 43, 1426-1429	1.3	91
104	First-Principles Calculations of Co Impurities and Native Defects in ZnO. *Materials Transactions*, **2002**, 43, 1439-1443	1.3	18
103	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
102	Theoretical Solution Energy of Alkaline Earth Ions in Lanthanum Chromites. *Materials Transactions*, **2002**, 43, 1456-1459	1.3	3
101	Growth of Bi-2212 single crystals by the travelling solvent zone melting method. *Superconductor Science and Technology*, **2002**, 15, 458-461	3.1	5
100	Transition behavior of La2CuO4+δ single crystals chemically oxidized in KMnO4 aqueous solution. *Physica C: Superconductivity and Its Applications*, **2001**, 357-360, 367-370	1.3	
99	Preparation of La2−xSrxCuO4 single-crystalline films by infrared-heated liquid phase epitaxial technique. *Physica C: Superconductivity and Its Applications*, **2001**, 362, 180-185	1.3	4
98	Josephson vortex flow in La2−xSrxCuO4 single crystals. *Physica C: Superconductivity and Its Applications*, **2001**, 362, 277-281	1.3	4
97	Subgap structures in the current–voltage properties of La2−xSrxCuO4 intrinsic Josephson junctions. *Physica C: Superconductivity and Its Applications*, **2001**, 362, 290-295	1.3	13
96	Control of the anisotropic growth rates of oxide single crystals in floating zone growth. *Journal of Crystal Growth*, **2001**, 229, 423-427	1.6	6
95	Intergranular Glassy Films in Ceramics.. *Journal of the Ceramic Society of Japan*, **2001**, 109, S127-S134		5
94	The effect of B2O3 addition on La2−xSrxCuO4 single-crystal growth. *Journal of Crystal Growth*, **2000**, 212, 138-141	1.6	8
93	X-ray topography investigation of La2−xSrxCuO4 single crystals. *Physica C: Superconductivity and Its Applications*, **2000**, 336, 244-248	1.3	4
92	Different tunneling regimes in La2−xSrxCuO4−δ break junctions. *Physica C: Superconductivity and Its Applications*, **2000**, 341-348, 1935-1936	1.3	
91	Superconductivity of hydrogen inserted LiNbO2. *Materials Research Bulletin*, **2000**, 35, 1743-1746	5.1	8
90	Chemical Bondings around Intercalated Cr and Fe Atoms in TiS2. *Materials Transactions, JIM*, **2000**, 41, 1088-1091		2

89	Chemical Oxidation on The Surface of La2CuO4 Single Crystals **2000**, 140-142		
88	Growth of La2−SrxCuO4 single-crystalline films by liquid phase epitaxial technique. *Physica C: Superconductivity and Its Applications*, **1999**, 315, 154-158	1.3	8
87	Valence Band Structure of ZnO (1010) Surface by Cluster Calculation **1999**, 4, 69-80		11
86	Electronic Mechanism of Ag-Cluster Formation in AgBr and AgI. *Journal of the Physical Society of Japan*, **1998**, 67, 2027-2036	1.5	19
85	Six-fold coordinated silicon at grain boundaries in sintered -Al2O3. *Applied Physics Letters*, **1998**, 72, 191-193	3.4	8
84	Electronic Structure and Chemical Bonding of TiS2 by Cluster Calculation. *Materials Transactions, JIM*, **1998**, 39, 709-713		6
83	TSFZ Growth of La2-xBaxCuO4 Single Crystals Under Varied Oxygen Partial Pressure **1998**, 371-374		1
82	Flux-line lock-in to CuO planes in a La1.9Sr0.1CuO4 single crystal. *Physical Review B*, **1997**, 56, 5610-5616	3.3	19
81	Effect of solute atoms on the chemical bonding of Fe3C (cementite). *The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties*, **1997**, 75, 237-248		25
80	Single crystal growth of superconducting La2−MxCuO4 (M?Ca, Sr, Ba) by the TSFZ method. *Physica C: Superconductivity and Its Applications*, **1997**, 293, 14-19	1.3	15
79	Fabrication of High-Jc Bi-2223 Sintered Bulk Superconductors. *Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals*, **1997**, 61, 900-905	0.4	7
78	Electronic States and Chemical Bondings of an Interstitial Cation in Ionic CompoundsAgCl and NaCl. *Journal of the Physical Society of Japan*, **1996**, 65, 3582-3590	1.5	22
77	First-principles molecular orbital calculation of electron energy-loss near-edge structures of -quartz. *Journal Physics D: Applied Physics*, **1996**, 29, 1725-1729	3	24
76	Electronic States of F-Centers in Alkali Halide Crystals. *Journal of the Physical Society of Japan*, **1996**, 65, 2564-2570	1.5	1
75	Orientation of the flux line lattice in anisotropic superconductors. *Journal of Magnetism and Magnetic Materials*, **1996**, 157-158, 671-672	2.8	1
74	Growth and superconductivity of La2−CaxCuO4 single crystals. *Physica C: Superconductivity and Its Applications*, **1996**, 262, 202-206	1.3	4
73	Raman-scattering study of CuGeO3. *Physica B: Condensed Matter*, **1996**, 219-220, 104-106	2.8	12
72	Anisotropic electric resistivity of superconducting La2−BaxCuO4 single crystals. *Physica C: Superconductivity and Its Applications*, **1996**, 258, 315-320	1.3	7

71	Crystal growth of pure and Zn-doped CuGeO3 by the floating zone (FZ) method. *Journal of Crystal Growth*, **1996**, 169, 469-473	1.6	5
70	Thermal Expansion Anomaly in High Tc La1.85Sr0.15CuO4 Associated with the Superconductivity **1996**, 219-222		
69	High-Temperature Fracture Mechanism of Low-Ca-Doped Silicon Nitride. *Journal of the American Ceramic Society*, **1995**, 78, 673-679	3.8	17
68	Faraday rotation and magnetization in CuGeO3 in ultra-high magnetic fields. *Physica B: Condensed Matter*, **1995**, 211, 184-186	2.8	9
67	Lattice-dynamics and spin-excitations in the spin-Peierls compound CuGeO3. *Physica B: Condensed Matter*, **1995**, 213-214, 284-287	2.8	6
66	Crystal growth of strontium-substituted barium titanate (Ba1⊠SrxTiO3) by the floating zone method. *Journal of Crystal Growth*, **1995**, 155, 70-74	1.6	14
65	Unconventional lattice stiffening in superconducting La2-xSrxCuO4 single crystals. *Physical Review B*, **1995**, 52, 570-580	3.3	75
64	Electronic structure of 3d transition elements in ⊞Si3N4. *The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties*, **1995**, 72, 459-473		6
63	Profile changes of X-ray spectra and their interpretation using the molecular-orbital method(Review).. *Bunseki Kagaku*, **1995**, 44, 251-269	0.2	11
62	Unusual Lattice Hardening below Tc in La2⊠SrxCuO4 **1995**, 219-224		
61	Homogeneity of Single Crystal of High-TcSuperconductorLa2-xSrxCuO4. *Japanese Journal of Applied Physics*, **1994**, 33, 4593-4597	1.4	2
60	Raman-scattering study of CuGeO3 in the spin-Peierls phase. *Physical Review B*, **1994**, 50, 16468-16474	3.3	88
59	Thermal contraction at the spin-Peierls transition in CuGeO3. *Physical Review B*, **1994**, 50, 12606-12610	3.3	46
58	Soft longitudinal modes in spin-singlet CuGeO3. *Physical Review B*, **1994**, 50, 1278-1281	3.3	109
57	Irreversibility boundaries of Bi2Sr2CaCu2O8, La1.86Sr0.14CuO4, and YBa2Cu3O7: An interpretation based on the vortex-lattice quantum-melting model. *Physica B: Condensed Matter*, **1994**, 194-196, 1555-1556	2.8	14
56	Elastic anomalies in a La1.85Sr0.15CuO4 single crystal under high magnetic fields. *Physica B: Condensed Matter*, **1994**, 194-196, 1579-1580	2.8	6
55	Anisotropy of the flux pinning in La1.85Sr0.15CuO4 observed by ultrasound. *Physica B: Condensed Matter*, **1994**, 194-196, 1837-1838	2.8	
54	The dependence of the magnetoacoustic properties of La2-xSrxCuO4 on doping. *Physica B: Condensed Matter*, **1994**, 194-196, 1863-1864	2.8	2

53	Electron irradiation effects on a La1.85Sr0.15CuO4 single crystal. *Physica B: Condensed Matter*, **1994**, 194-196, 1881-1882	2.8	4
52	Effects of superconductivity on elastic constants of La2−SrxCuO4. *Physica B: Condensed Matter*, **1994**, 194-196, 2167-2168	2.8	4
51	Anisotropic electrical resistivity and oxygen annealing effect on it in La2−CaxCuO4 single crystals. *Physica C: Superconductivity and Its Applications*, **1994**, 234, 115-119	1.3	3
50	Single-crystal growth of Nd2−CexCuO4 at low oxygen pressure in ambient atmosphere. *Physica C: Superconductivity and Its Applications*, **1994**, 228, 58-62	1.3	4
49	The dependence of Ce incorporation on the effective distribution coefficient of Ce in Nd2−CexCuO4 single crystals grown by the TSFZ method. *Physica C: Superconductivity and Its Applications*, **1994**, 226, 262-266	1.3	2
48	Determination of the solubility of alkaline-earth metals (Ca, Sr, Ba) into La2CuO4 by the SCFZ method. *Physica C: Superconductivity and Its Applications*, **1994**, 225, 185-189	1.3	11
47	Relation between structure and doping in La2−SrxCuO4+δ a neutron diffraction study on single crystals. *Physica C: Superconductivity and Its Applications*, **1994**, 223, 396-416	1.3	46
46	TSFZ growth of Nd2-xCexCuO4 single crystals at low oxygen pressure. *Physica C: Superconductivity and Its Applications*, **1994**, 235-240, 557-558	1.3	2
45	Thermal expansion of a La1.87Sr0.13CuO4 single crystal at Tc in high magnetic fields. *Physica C: Superconductivity and Its Applications*, **1994**, 235-240, 1931-1932	1.3	1
44	Elastic and inelastic neutron scattering studies on the tetragonal to orthorhombic phase transition of La2− Sr x CuO4−δ *European Physical Journal B*, **1994**, 94, 29-37	1.2	23
43	Crystal growth of high Sr-doped La2-xSrxCuO4 by the TSFZ method **1994**, 353-356		
42	Characterization of Single Crystals of High-TcSuperconductor La2-xSrxCuO4. *Japanese Journal of Applied Physics*, **1993**, 32, 4959-4965	1.4	2
41	Interplay between lattice softening and high-Tc superconductivity in La1.86Sr0.14CuO4. *Physical Review Letters*, **1993**, 70, 3447-3450	7.4	67
40	Elastic properties and anisotropic pinning of the flux-line lattice in single-crystalline La1.85Sr0.15CuO4. *Physical Review B*, **1993**, 48, 9772-9781	3.3	21
39	Low-Energy Spin Fluctuations inLa2-xSrxCu1-yZnyO4(x=0.14,y=0.012). *Journal of the Physical Society of Japan*, **1993**, 62, 443-446	1.5	23
38	Single crystal growth of pure and Y-substituted NdAlO3 by the floating zone (FZ) method. *Journal of Crystal Growth*, **1993**, 128, 680-683	1.6	2
37	Cerium distribution coefficient and its dependence on oxygen partial pressure in Nd2−CexCuO4 single crystal growth. *Physica C: Superconductivity and Its Applications*, **1993**, 218, 437-442	1.3	6
36	Temperature dependence of (□) paramagnetic shift in highT c superconductor La2− Sr x CuO4. *Hyperfine Interactions*, **1993**, 79, 879-883	0.8	6

35	Local hyperfine field vector of positive muon in mono-domain single crystal of antiferromagnetic La2CuO4. *Hyperfine Interactions*, **1993**, 79, 915-920	0.8	6
34	Behavior of positive muons in highT c superconductors La2 Sr x CuO4. *Hyperfine Interactions*, **1993**, 79, 921-927	0.8	17
33	Optical studies on La2SrxCuO4single crystals. *Physica C: Superconductivity and Its Applications*, **1992**, 193, 277-290	1.3	11
32	Characterization and structural analysis of twinned La2SrxCuO4crystals by neutron diffraction. *Physica C: Superconductivity and Its Applications*, **1992**, 191, 455-468	1.3	31
31	A New Method of Determining Tc(H) of Single-Crystal La2SrxCuO4 from the Field-Dependent Susceptibility Above Tc **1992**, 159-162		
30	Neutron depolarization study of flux distribution in superconducting state. *Physica C: Superconductivity and Its Applications*, **1991**, 185-189, 1839-1840	1.3	1
29	Anisotropic susceptibility in the normal state and superconducting fluctuation-induced diamagnetism of single-crystal La2SraCuO4. *Physica C: Superconductivity and Its Applications*, **1991**, 185-189, 1855-1856	1.3	7
28	Quantitative analysis of zero field cooling and field cooling curves to determine the critical current density and lower critical field. *Physica C: Superconductivity and Its Applications*, **1991**, 185-189, 2163-2164	1.3	2
27	Optical properties and transition temperatures of La2SrxCuO4 crystals (x=0, 0.14, 0.19). *Physica C: Superconductivity and Its Applications*, **1991**, 185-189, 951-952	1.3	
26	Thermal expansion measurements in a La1.85Sr0.15CuO4 single crystal superconductor by X-ray diffraction. *Physica C: Superconductivity and Its Applications*, **1991**, 185-189, 1383-1384	1.3	7
25	Ultrasonic studies in the La1.85Sr0.15CuO4 single crystal under the magnetic field. *Physica C: Superconductivity and Its Applications*, **1991**, 185-189, 1395-1396	1.3	9
24	Anisotropic coupling between high-Tc superconductivity and lattice in single-crystalline La1.86Sr0.14CuO4. *Physica C: Superconductivity and Its Applications*, **1991**, 185-189, 1397-1398	1.3	10
23	Growth and superconductivity of Nd2CexCuO4 single crystals. *Physica C: Superconductivity and Its Applications*, **1991**, 185-189, 437-438	1.3	17
22	Muon spin relaxation study on magnetism in high quality single crystal of a high transition temperature superconductor La2SrxCuO4(0.11.14). *Hyperfine Interactions*, **1991**, 63, 271-277	0.8	30
21	Probing oxygen in high Tc superconductor LaSrCuO by negative muons. *Hyperfine Interactions*, **1991** , 65, 1015-1026	0.8	5
20	Phase equilibrium in the NdCeCuO system. *Physica C: Superconductivity and Its Applications*, **1991**, 190, 112-113	1.3	13
19	Growth and Superconductive Properties of La2CuO4 Single Crystals **1991**, 455-458		
18	Anisotropy in Magnetization and Critical Current Density of La-Sr-Cu-O Single Crystal **1991**, 563-566		

17	Single crystal growth of pure and Ba-doped strontium tantalate (SrTa206) by floating zone method. *Journal of Crystal Growth*, **1990**, 99, 837-840	1.6	7
16	Anisotropy of upper critical field in the (110)t and (001)t planes for single-crystal La1.86Sr0.14CuO4. *Physica B: Condensed Matter*, **1990**, 165-166, 1449-1450	2.8	23
15	Temperature dependence of anisotropic lower critical fields in (La1-xSrx)2CuO4. *Physical Review B*, **1990**, 41, 4823-4826	3.3	73
14	Inelastic-neutron-scattering study of the electron-phonon interaction in a superconducting La1.85Sr0.15CuO4 single crystal. *Physical Review B*, **1990**, 42, 4272-4275	3.3	6
13	Complete elastic constants and giant softening of c66 in superconducting La1.86Sr0.14CuO4. *Physical Review Letters*, **1990**, 64, 2458-2461	7.4	77
12	The Growth of Nd2-xCexCuO4 Single Crystals by the TSFZ Method. *Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics*, **1990**, 184, 69-73		1
11	Broadening Mechanism of Resistive Transition under Magnetic Field in Single Crystalline (La1-xSrx)2CuO4. *Japanese Journal of Applied Physics*, **1989**, 28, L555-L556	1.4	109
10	Preparation of Y-Ba-Cu-O Superconducting Thin Films by the Mist Microwave Plasma Decomposition Method. *Japanese Journal of Applied Physics*, **1989**, 28, L1212-L1213	1.4	24
9	+ SR lineshape of oriented and unoriented high T c superconductors. *Physica C: Superconductivity and Its Applications*, **1989**, 162-164, 1555-1556	1.3	7
8	Single crystal growth of superconducting La2-xSrxCuO4 by the TSFZ method. *Journal of Crystal Growth*, **1989**, 96, 711-715	1.6	85
7	Dielectric properties of BaTi4O9 single crystals. *Journal of Materials Science*, **1989**, 24, 959-962	4.3	8
6	Growth of Superconducting La2SrxCuO4 Single Crystals. *Materials Research Society Symposia Proceedings*, **1989**, 156, 183		
5	Growth and characterization of titanite (CaTiSiO5) single crystals by the floating zone method. *Journal of Crystal Growth*, **1988**, 87, 169-174	1.6	18
4	Single crystal growth of tantalite ((Fe,Mn)(Ta,Nb)2O6) solid solutions. *Journal of Crystal Growth*, **1988**, 91, 141-146	1.6	3
3	The growth of barium tetratitanate (BaTi4O9) single crystals by the floating zone method. *Journal of Crystal Growth*, **1986**, 76, 311-316	1.6	5
2	The growth of tapiolite (FeTa2O6) single crystals by the floating zone method. *Journal of Crystal Growth*, **1985**, 73, 175-178	1.6	6
1	Poster: Electronic Structure, Lattice Dynamics, and Transport471-522		