Isao Tanaka

List of Publications by Year in Descending Order

351 papers	23,155 citations	65 h-index	143 g-index
364 ext. papers	27,000 ext. citations	4.2 avg, IF	7.51 L-index

#	Paper	IF	Citations
351	Proposing the Concept of Plaston and Strategy to Manage Both High Strength and Large Ductility in Advanced Structural Materials, on the Basis of Unique Mechanical Properties of Bulk Nanostructured Metals **2022**, 3-34		1
350	Collective Motion of Atoms in Metals by First Principles Calculations **2022**, 79-90		
349	Combination of recommender system and single-particle diagnosis for accelerated discovery of novel nitrides. *Journal of Chemical Physics*, **2021**, 154, 224117	3.9	1
348	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
347	Fast material search of lithium ion conducting oxides using a recommender system. *Journal of Materials Chemistry A*, **2020**, 8, 11582-11588	13	11
346	Strategy for managing both high strength and large ductility in structural materials: Sequential nucleation of different deformation modes based on a concept of plaston. *Scripta Materialia*, **2020**, 181, 35-42	5.6	27
345	Application of machine learning potentials to predict grain boundary properties in fcc elemental metals. *Physical Review Materials*, **2020**, 4,	3.2	11
344	Recommender Systems for Materials Discovery. *Lecture Notes in Physics*, **2020**, 427-443	0.8	
343	Data-Driven Materials Discovery from Large Chemistry Spaces. *Matter*, **2020**, 3, 327-328	12.7	1
342	Enumeration of nonequivalent substitutional structures using advanced data structure of binary decision diagram. *Journal of Chemical Physics*, **2020**, 153, 104109	3.9	0
341	First-Principles Study on the Stability of Weberite-Type, Pyrochlore, and Defect-Fluorite Structures of A23+B24+O7 (A = Lu3+La3+, B = Zr4+, Hf4+, Sn4+, and Ti4+). *Journal of Physical Chemistry C*, **2020**, 124, 20555-20562	3.8	3
340	Group-theoretical high-order rotational invariants for structural representations: Application to linearized machine learning interatomic potential. *Physical Review B*, **2019**, 99,	3.3	19
339	Equilibrium hydrogen pressures in the VH system from first principles. *International Journal of Hydrogen Energy*, **2019**, 44, 28909-28918	6.7	5
338	Prediction of dielectric constants using a combination of first principles calculations and machine learning. *Japanese Journal of Applied Physics*, **2019**, 58, SLLC01	1.4	9
337	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
336	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
335	Vibrational Effects in X-ray Absorption Spectra of Two-Dimensional Layered Materials. *Journal of Physical Chemistry C*, **2019**, 123, 9688-9692	3.8	5

334	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
333	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
332	Finite-displacement computation of the electron-phonon interaction within the projector augmented-wave method. *Physical Review B*, **2019**, 100,	3.3	6
331	Design and synthesis of a magnesium alloy for room temperature hydrogen storage. *Acta Materialia*, **2018**, 149, 88-96	8.4	101
330	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
329	Descriptors for Machine Learning of Materials Data **2018**, 3-23		26
328	Compositional descriptor-based recommender system for the materials discovery. *Journal of Chemical Physics*, **2018**, 148, 241719	3.9	22
327	Temperature-dependent phonon spectra of magnetic random solid solutions. *Npj Computational Materials*, **2018**, 4,	10.9	13
326	Bulk nanocrystalline gamma magnesium hydride with low dehydrogenation temperature stabilized by plastic straining via high-pressure torsion. *Scripta Materialia*, **2018**, 157, 54-57	5.6	19
325	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
324	Double thermoelectric power factor of a 2D electron system. *Nature Communications*, **2018**, 9, 2224	17.4	35
323	Matrix- and tensor-based recommender systems for the discovery of currently unknown inorganic compounds. *Physical Review Materials*, **2018**, 2,	3.2	29
322	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
321	Synthesis, crystal structure, and ionic conductivity of hydride ion-conducting Ln2LiHO3 (Ln = La, Pr, Nd) oxyhydrides. *Journal of Materials Chemistry A*, **2018**, 6, 23457-23463	13	16
320	Materials informatics for dielectric materials. *Japanese Journal of Applied Physics*, **2018**, 57, 11UB01	1.4	9
319	High Rate Performance of Dual-Substituted LiFePO4 Based on Controlling Metastable Intermediate Phase. *ACS Applied Energy Materials*, **2018**, 1, 6736-6740	6.1	5
318	Data-centric science for materials innovation. *MRS Bulletin*, **2018**, 43, 659-663	3.2	17
317	Impact of Chemical Fluctuations on Stacking Fault Energies of CrCoNi and CrMnFeCoNi High Entropy Alloys from First Principles. *Entropy*, **2018**, 20,	2.8	42

316	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
315	Thermoelectric phase diagram of the SrTiO3–SrNbO3 solid solution system. *Journal of Applied Physics*, **2017**, 121, 185102	2.5	15
314	Theoretical investigation of solid solution states of Ti1−xVxH2. *Acta Materialia*, **2017**, 134, 274-282	8.4	2
313	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
312	Mode decomposition based on crystallographic symmetry in the band-unfolding method. *Physical Review B*, **2017**, 95,	3.3	23
311	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
310	Band structure diagram paths based on crystallography. *Computational Materials Science*, **2017**, 128, 140-184	3.2	247
309	Materials Design Using First-Principles Calculations for Lithium-Ion Batteries. *Materia Japan*, **2017**, 56, 430-433	0.1	
308	DynaPhoPy: A code for extracting phonon quasiparticles from molecular dynamics simulations. *Computer Physics Communications*, **2017**, 221, 221-234	4.2	48
307	Comparison of approximations in density functional theory calculations: Energetics and structure of binary oxides. *Physical Review B*, **2017**, 96,	3.3	58
306	Representation of compounds for machine-learning prediction of physical properties. *Physical Review B*, **2017**, 95,	3.3	158
305	Atomistic Origin of Phase Stability in Oxygen-Functionalized MXene: A Comparative Study. *Journal of Physical Chemistry C*, **2017**, 121, 18947-18953	3.8	34
304	First-principles screening of structural properties of intermetallic compounds on martensitic transformation. *Npj Computational Materials*, **2017**, 3,	10.9	9
303	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
302	Band alignment of semiconductors and insulators using dielectric-dependent hybrid functionals: Toward high-throughput evaluation. *Physical Review B*, **2017**, 95,	3.3	45
301	Discovery of a Novel Sn(II)-Based Oxide SnMoO for Daylight-Driven Photocatalysis. *Advanced Science*, **2017**, 4, 1600246	13.6	18
300	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
299	Anharmonicity in the High-Temperature Cmcm Phase of SnSe: Soft Modes and Three-Phonon Interactions. *Physical Review Letters*, **2016**, 117, 075502	7.4	104

298	Low phonon conductivity of layered BiCuOS, BiCuOSe, and BiCuOTe from first principles. *Physical Review B*, **2016**, 94,	3.3	17
297	Stability of the structure of transition elements. *Physical Review B*, **2016**, 93,	3.3	15
296	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
295	Discovery of earth-abundant nitride semiconductors by computational screening and high-pressure synthesis. *Nature Communications*, **2016**, 7, 11962	17.4	133
294	Categorization of surface polarity from a crystallographic approach. *Computational Materials Science*, **2016**, 113, 221-230	3.2	31
293	structure in steel: A first-principles study. *Journal of Alloys and Compounds*, **2016**, 684, 624-627	5.7	16
292	Pure H? conduction in oxyhydrides. *Science*, **2016**, 351, 1314-7	33.3	110
291	New nanostructured phases with reversible hydrogen storage capability in immiscible magnesium zirconium system produced by high-pressure torsion. *Acta Materialia*, **2016**, 108, 293-303	8.4	54
290	Toward Materials Discovery with First-Principles Datasets and Learning Methods. *Springer Series in Materials Science*, **2016**, 173-186	0.9	
289	Complex Point Defect Structure in Cubic Boron Nitride. *Materia Japan*, **2016**, 55, 609-609	0.1	
288	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
287	Suppression of lattice thermal conductivity by mass-conserving cation mutation in multi-component semiconductors. *APL Materials*, **2016**, 4, 104809	5.7	8
286	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
285	Electronic Structure and Defect Chemistry of Tin(II) Complex Oxide SnNb2O6. *Journal of Physical Chemistry C*, **2016**, 120, 9604-9611	3.8	19
284	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
283	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
282	Distributions of phonon lifetimes in Brillouin zones. *Physical Review B*, **2015**, 91,	3.3	607
281	Li Intercalation into a MnO2 Grain Boundary. *ACS Applied Materials & Interfaces*, **2015**, 7, 8125-31	9.5	14

280	Special quasirandom structure in heterovalent ionic systems. *Physical Review B*, **2015**, 91,	3.3	5
279	First principles phonon calculations in materials science. *Scripta Materialia*, **2015**, 108, 1-5	5.6	4076
278	First-principles interatomic potentials for ten elemental metals via compressed sensing. *Physical Review B*, **2015**, 92,	3.3	52
277	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
276	Stability of 12CaO·7Al2O3 Crystal under High-Pressure: Experimental and First-Principles Approaches. *Materials Transactions*, **2015**, 56, 1350-1353	1.3	3
275	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
274	Selective fabrication of n- and p-type SnO films without doping. *Physica Status Solidi - Rapid Research Letters*, **2015**, 9, 192-196	2.5	16
273	Proton trapping in Y and Sn Co-doped BaZrO3. *Journal of Materials Chemistry A*, **2015**, 3, 10045-10051	13	24
272	First principles study of thermal conductivity cross-over in nanostructured zinc-chalcogenides. *Journal of Applied Physics*, **2015**, 117, 045102	2.5	20
271	Epitaxial growth of tin(II) niobate with a pyrochlore structure. *Journal of Crystal Growth*, **2015**, 416, 126-129	1.9	4
270	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
269	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
268	Inversion symmetry breaking by oxygen octahedral rotations in the Ruddlesden-Popper NaRTiO4 family. *Physical Review Letters*, **2014**, 112, 187602	7.4	45
267	Photocatalytic activity of □PbO2-type TiO2. *Physica Status Solidi - Rapid Research Letters*, **2014**, 8, 822-826	2.5	12
266	Local Structure and Energetics of Pr- and La-Doped SrTiO3 Grain Boundaries and the Influence on Core□Shell Structure Formation. *Journal of Physical Chemistry C*, **2014**, 118, 25765-25778	3.8	17
265	Efficient determination of alloy ground-state structures. *Physical Review B*, **2014**, 90,	3.3	9
264	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
263	First principles study of dopant solubility and defect chemistry in LiCoO2. *Journal of Materials Chemistry A*, **2014**, 2, 11235-11245	13	46

262	Phonon softening in paramagnetic bcc Fe and its relationship to the pressure-induced phase transition. *Physical Review B*, **2014**, 90,	3.3	29
261	Proton incorporation and trapping in ZrO2 grain boundaries. *Journal of Materials Chemistry A*, **2014**, 2, 1400-1408	13	17
260	Accelerated discovery of cathode materials with prolonged cycle life for lithium-ion battery. *Nature Communications*, **2014**, 5, 4553	17.4	86
259	Significant reduction in hydration energy for yttria stabilized zirconia grain boundaries and the consequences for proton conduction. *Langmuir*, **2014**, 30, 10456-64	4	8
258	Surface design of alloy protection against CO-poisoning from first principles. *Journal of Physics Condensed Matter*, **2014**, 26, 355006	1.8	2
257	Protonic defects in yttria stabilized zirconia: incorporation, trapping and migration. *Physical Chemistry Chemical Physics*, **2014**, 16, 4814-22	3.6	13
256	Thermal physics of the lead chalcogenides PbS, PbSe, and PbTe from first principles. *Physical Review B*, **2014**, 89,	3.3	172
255	Atomic structure of luminescent centers in high-efficiency Ce-doped w-AlN single crystal. *Scientific Reports*, **2014**, 4, 3778	4.9	34
254	Mn L2,3-edge X-ray absorption spectroscopic studies on charge-discharge mechanism of Li2MnO3. *Applied Physics Letters*, **2014**, 104, 053906	3.4	37
253	Sparse representation for a potential energy surface. *Physical Review B*, **2014**, 90,	3.3	59
252	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
251	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
250	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
249	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
248	Strong Spin-Lattice Coupling Through Oxygen Octahedral Rotation in Divalent Europium Perovskites. *Advanced Functional Materials*, **2013**, 23, 1864-1872	15.6	28
247	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
246	Functional complex point-defect structure in a huge-size-mismatch system. *Physical Review Letters*, **2013**, 110, 065504	7.4	33
245	Anti-ferrodistortive-like oxygen-octahedron rotation induced by the oxygen vacancy in cubic SrTiO3. *Advanced Materials*, **2013**, 25, 86-90	24	76

244	Variation of Zr-L2,3 XANES in tetravalent zirconium oxides. *Journal of Physics Condensed Matter*, **2013**, 25, 165505	1.8	15
243	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
242	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
241	Evolution of crystal structures in metallic elements. *Physical Review B*, **2013**, 87,	3.3	56
240	Valence band offsets at zinc-blende heterointerfaces with misfit dislocations: A first-principles study. *Physical Review B*, **2013**, 88,	3.3	10
239	Band offsets of CuInSe2/CdS and CuInSe2/ZnS (110) interfaces: A hybrid density functional theory study. *Physical Review B*, **2013**, 88,	3.3	38
238	Theoretical Photovoltaic Conversion Efficiencies of ZnSnP2, CdSnP2, and Zn1-xCdxSnP2Alloys. *Applied Physics Express*, **2013**, 6, 061201	2.4	31
237	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
236	Local environment of silicon in cubic boron nitride. *Journal of Applied Physics*, **2013**, 114, 233502	2.5	10
235	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
234	Co K-edge XANES of LiCoO2 and CoO2 with a variety of structures by supercell density functional calculations with a core hole. *Physical Review B*, **2012**, 85,	3.3	21
233	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
232	Ionization potentials of (112) and (112□) facet surfaces of CuInSe2 and CuGaSe2. *Physical Review B*, **2012**, 86,	3.3	59
231	Nitrogen and hydrogen defect equilibria in Ca12Al14O33: a combined experimental and computational study. *Journal of Materials Chemistry*, **2012**, 22, 15828		13
230	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
229	Proton-Conducting Network in Lanthanum Orthophosphate. *Journal of Physical Chemistry C*, **2012**, 116, 19117-19124	3.8	38
228	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
227	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

226	Ground-state search in multicomponent magnetic systems. *Physical Review B*, **2012**, 85,	3.3	3
225	First-principles calculations of the phase diagrams and band gaps in CuInSe2-CuGaSe2 and CuInSe2-CuAlSe2 pseudobinary systems. *Physical Review B*, **2012**, 85,	3.3	31
224	Tetravalent dysprosium in a perovskite-type oxide. *Advanced Materials*, **2012**, 24, 2051-3	24	20
223	Cluster expansion with controlled accuracy for the MgO/ZnO pseudobinary system via first-principles calculations. *Physical Review B*, **2012**, 86,	3.3	9
222	Site preference of cation vacancies in Mn-doped Ga2O3 with defective spinel structure. *Applied Physics Letters*, **2012**, 101, 241906	3.4	8
221	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
220	Point defects in ZnO: an approach from first principles. *Science and Technology of Advanced Materials*, **2011**, 12, 034302	7.1	234
219	Grouping of structures for cluster expansion of multicomponent systems with controlled accuracy. *Physical Review B*, **2011**, 83,	3.3	13
218	Atomic and electronic structures of the SrVO3-LaAlO3 interface. *Journal of Applied Physics*, **2011**, 110, 046104	2.5	14
217	First-principles calculations of lattice dynamics in CdTiO3 and CaTiO3: Phase stability and ferroelectricity. *Physical Review B*, **2011**, 84,	3.3	47
216	First-principles thermodynamics of La2O3-P2O5 pseudobinary system. *Physical Review B*, **2011**, 84,	3.3	14
215	Hybrid density functional study of oxygen vacancies in KTaO3 and NaTaO3. *Physical Review B*, **2011**, 83,	3.3	23
214	Atomistic structure and energetics of interface between Mn-doped □Ga2O3 and MgAl2O4. *Journal of Materials Science*, **2011**, 46, 4169-4175	4.3	9
213	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
212	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
211	Electronic and structural properties of the oxygen vacancy in BaTiO3. *Applied Physics Letters*, **2011**, 98, 172901	3.4	49
210	Electronic structures of dynamically stable As2O3, Sb2O3, and Bi2O3 crystal polymorphs. *Physical Review B*, **2011**, 83,	3.3	33
209	Synthesis and electrochemistry of monoclinic Li(MnxFe1□)BO3: a combined experimental and computational study. *Journal of Materials Chemistry*, **2011**, 21, 10690		45

208	Phonon-phonon interactions in transition metals. *Physical Review B*, **2011**, 84,	3.3	235
207	Alkali-metal adsorption and manipulation on a hydroxylated TiO2(110) surface using atomic force microscopy. *Physical Review B*, **2011**, 84,	3.3	18
206	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
205	Epitaxial growth of Mn-doped Ga2O3 on spinel substrate. *Journal of Materials Research*, **2011**, 26, 578-583	2.3	35
204	Doping of hexagonal boron nitride via intercalation: A theoretical prediction. *Physical Review B*, **2010**, 81,	3.3	53
203	First-principles phonon calculations of thermal expansion in Ti3SiC2, Ti3AlC2, and Ti3GeC2. *Physical Review B*, **2010**, 81,	3.3	309
202	Anisotropic phonon density of states in FePt nanoparticles with L10 structure. *Physical Review B*, **2010**, 81,	3.3	9
201	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
200	Process-Induced Damage Characterization of Patterned Low- Film Using Electron Energy Loss Spectroscopy Technique. *Japanese Journal of Applied Physics*, **2010**, 49, 111501	1.4	1
199	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
198	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
197	Classification of spinel structures based on first-principles cluster expansion analysis. *Physical Review B*, **2010**, 81,	3.3	27
196	Thermodynamics and structures of oxide crystals by a systematic set of first principles calculations. *Journal of Materials Chemistry*, **2010**, 20, 10335		7
195	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
194	First-principles calculations of Zn-K XANES in Ca-deficient hydroxyapatite. *Journal of Physics Condensed Matter*, **2010**, 22, 384213	1.8	11
193	Native defects in oxide semiconductors: a density functional approach. *Journal of Physics Condensed Matter*, **2010**, 22, 384211	1.8	41
192	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
191	Lithium iron borates as high-capacity battery electrodes. *Advanced Materials*, **2010**, 22, 3583-7	24	204

190	Theoretical ELNES using one-particle and multi-particle calculations. *Micron*, **2010**, 41, 695-709	2.3	72
189	Magnetic properties of ilmenite-hematite solid-solution thin films: Direct observation of antiphase boundaries and their correlation with magnetism. *Physical Review B*, **2009**, 80,	3.3	9
188	First-principles prediction of low-energy structures for AlH3. *Physical Review B*, **2009**, 79,	3.3	7
187	Variable anisotropy of ionic conduction in lithium nitride: Effect of duplex-charge transfer. *Physical Review B*, **2009**, 80,	3.3	4
186	First-principles study of defect-induced potentials in Ca2CuO2Cl2. *Physical Review B*, **2009**, 80,	3.3	5
185	Role of Ti antisitelike defects in SrTiO3. *Physical Review Letters*, **2009**, 103, 185502	7.4	90
184	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
183	Multiplet calculations of L(2,3) x-ray absorption near-edge structures for 3d□transition-metal compounds. *Journal of Physics Condensed Matter*, **2009**, 21, 104208	1.8	94
182	All-electron CI calculations of 3d transition-metal L(2,3) XANES using zeroth-order regular approximation for relativistic effects. *Journal of Physics Condensed Matter*, **2009**, 21, 104209	1.8	4
181	First-principles calculation of spectral features, chemical shift and absolute threshold of ELNES and XANES using a plane wave pseudopotential method. *Journal of Physics Condensed Matter*, **2009**, 21, 104204	1.8	68
180	Lattice dynamics and thermal properties of SrHfO3 by first-principles calculations. *Physica Status Solidi (B): Basic Research*, **2009**, 246, 1628-1633	1.3	9
179	First-principles study on lithium removal from Li2MnO3. *Journal of Power Sources*, **2009**, 189, 798-801	8.9	136
178	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
177	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
176	First Principles Thermodynamics Calculations of Atomic Scale Modifications. *Materia Japan*, **2009**, 48, 299-302	0.1	
175	First Principles Lattice Dynamics Calculations of Ag+ Doped KX (X=Cl, Br and I). *Materials Transactions*, **2009**, 50, 999-1003	1.3	
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