Isao Tanaka

List of Publications by Citations

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	First principles phonon calculations in materials science. *Scripta Materialia*, **2015**, 108, 1-5	5.6	4076
350	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
349	High-density electron anions in a nanoporous single crystal: [Ca24Al28O64]4+(4e-). *Science*, **2003**, 301, 626-9	33.3	638
348	Defect energetics in ZnO: A hybrid Hartree-Fock density functional study. *Physical Review B*, **2008**, 77,	3.3	613
347	Distributions of phonon lifetimes in Brillouin zones. *Physical Review B*, **2015**, 91,	3.3	607
346	Energetics of native defects in ZnO. *Journal of Applied Physics*, **2001**, 90, 824-828	2.5	330
345	First-principles phonon calculations of thermal expansion in Ti3SiC2, Ti3AlC2, and Ti3GeC2. *Physical Review B*, **2010**, 81,	3.3	309
344	Crystal and electronic structures of superstructural Li1−[Co1/3Ni1/3Mn1/3]O2 (0−1). *Journal of Power Sources*, **2003**, 119-121, 644-648	8.9	284
343	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
342	Band structure diagram paths based on crystallography. *Computational Materials Science*, **2017**, 128, 140-184	3.2	247
341	Phonon-phonon interactions in transition metals. *Physical Review B*, **2011**, 84,	3.3	235
340	Point defects in ZnO: an approach from first principles. *Science and Technology of Advanced Materials*, **2011**, 12, 034302	7.1	234
339	Lithium iron borates as high-capacity battery electrodes. *Advanced Materials*, **2010**, 22, 3583-7	24	204
338	Interesting Physical Properties of the New Spinel Phase of Si3N4 and C3N4. *Physical Review Letters*, **1999**, 83, 5046-5049	7.4	192
337	Debye temperature and stiffness of carbon and boron nitride polymorphs from first principles calculations. *Physical Review B*, **2006**, 73,	3.3	181
336	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
335	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

334	Thermal physics of the lead chalcogenides PbS, PbSe, and PbTe from first principles. *Physical Review B*, **2014**, 89,	3.3	172
333	Hot Isostatic Press Sintering and Properties of Silicon Nitride without Additives. *Journal of the American Ceramic Society*, **1989**, 72, 1656-1660	3.8	162
332	First-principles approach to chemical diffusion of lithium atoms in a graphite intercalation compound. *Physical Review B*, **2008**, 78,	3.3	160
331	Representation of compounds for machine-learning prediction of physical properties. *Physical Review B*, **2017**, 95,	3.3	158
330	Calcium Concentration Dependence of the Intergranular Film Thickness in Silicon Nitride. *Journal of the American Ceramic Society*, **1994**, 77, 911-914	3.8	156
329	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
328	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
327	Solid-State Chemistry and Electrochemistry of LiCo[sub 1/3]Ni[sub 1/3]Mn[sub 1/3]O[sub 2] for Advanced Lithium-Ion Batteries. *Journal of the Electrochemical Society*, **2004**, 151, A1545	3.9	140
326	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
325	First-principles study on lithium removal from Li2MnO3. *Journal of Power Sources*, **2009**, 189, 798-801	8.9	136
324	Discovery of earth-abundant nitride semiconductors by computational screening and high-pressure synthesis. *Nature Communications*, **2016**, 7, 11962	17.4	133
323	Structure and stability of a homologous series of tin oxides. *Physical Review Letters*, **2008**, 100, 045702	7.4	129
322	Pure H? conduction in oxyhydrides. *Science*, **2016**, 351, 1314-7	33.3	110
321	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
320	Anharmonicity in the High-Temperature Cmcm Phase of SnSe: Soft Modes and Three-Phonon Interactions. *Physical Review Letters*, **2016**, 117, 075502	7.4	104
319	XANES and ELNES in Ceramic Science. *Journal of the American Ceramic Society*, **2005**, 88, 2013-2029	3.8	104
318	Design and synthesis of a magnesium alloy for room temperature hydrogen storage. *Acta Materialia*, **2018**, 149, 88-96	8.4	101
317	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

316	Electronic structure of lithium nickel oxides by electron energy loss spectroscopy. *Journal of Physical Chemistry B*, **2005**, 109, 10749-55	3.4	93
315	Decomposition reactions for NaAlH4, Na3AlH6, and NaH: First-principles study. *Physical Review B*, **2005**, 71,	3.3	93
314	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
313	Systematic Research on Insertion Materials Based on Superlattice Models in a Phase Triangle of LiCoO[sub 2]-LiNiO[sub 2]-LiMnO[sub 2]. *Journal of the Electrochemical Society*, **2004**, 151, A1499	3.9	92
312	Pressure-induced phase transition in ZnO and ZnO–MgO pseudobinary system: A first-principles lattice dynamics study. *Physical Review B*, **2005**, 72,	3.3	91
311	Theoretical Formation Energy of Oxygen-Vacancies in Oxides. *Materials Transactions*, **2002**, 43, 1426-1429	2.3	91
310	Role of Ti antisitelike defects in SrTiO3. *Physical Review Letters*, **2009**, 103, 185502	7.4	90
309	Ab initio lattice dynamics and phase transformations of ZrO2. *Physical Review B*, **2005**, 71,	3.3	90
308	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
307	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
306	First-principles XANES simulations of spinel zinc ferrite with a disordered cation distribution. *Physical Review B*, **2007**, 75,	3.3	88
305	Accelerated discovery of cathode materials with prolonged cycle life for lithium-ion battery. *Nature Communications*, **2014**, 5, 4553	17.4	86
304	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
303	First-principles multielectron calculations of Ni L2,3 NEXAFS and ELNES for LiNiO2 and related compounds. *Physical Review B*, **2005**, 72,	3.3	86
302	Theoretical Prediction of the Structure and Properties of Cubic Spinel Nitrides. *Journal of the American Ceramic Society*, **2004**, 85, 75-80	3.8	86
301	Reduced SnO2 surfaces by first-principles calculations. *Applied Physics Letters*, **2004**, 84, 909-911	3.4	85
300	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
299	Room temperature ferromagnetism in Mn-doped Ga2O3 with spinel structure. *Applied Physics Letters*, **2006**, 89, 181903	3.4	84

298	Prediction of spinel structure and properties of single and double nitrides. *Physical Review B*, **2001**, 63,	3.3	84
297	Mechanism of electrical conductivity of transparent InGaZnO4. *Physical Review B*, **2000**, 61, 1811-1816	3.3	83
296	Anti-ferrodistortive-like oxygen-octahedron rotation induced by the oxygen vacancy in cubic SrTiO3. *Advanced Materials*, **2013**, 25, 86-90	24	76
295	Calculation of core-hole excitonic features on Al L23-edge x-ray-absorption spectra of alpha -Al2O3. *Physical Review B*, **1996**, 54, 4604-4608	3.3	74
294	Theoretical ELNES using one-particle and multi-particle calculations. *Micron*, **2010**, 41, 695-709	2.3	72
293	Prediction of ground-state structures and order-disorder phase transitions in II-III spinel oxides: A combined cluster-expansion method and first-principles study. *Physical Review B*, **2006**, 73,	3.3	72
292	Identification of ultradilute dopants in ceramics. *Nature Materials*, **2003**, 2, 541-5	27	72
291	Lattice dynamics and thermodynamical properties of silicon nitride polymorphs. *Physical Review B*, **2008**, 78,	3.3	71
290	Calculation of multiplet structures of Cr3+ and V3+ in α-Al2O3 based on a hybrid method of density-functional theory and the configuration interaction. *Physical Review B*, **2000**, 61, 143-161	3.3	70
289	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
288	First-principles study of bulk ordering and surface segregation in Pt-Rh binary alloys. *Physical Review B*, **2006**, 74,	3.3	65
287	Cubic and orthorhombic structures of aluminum hydride AlH3 predicted by a first-principles study. *Physical Review B*, **2005**, 71,	3.3	65
286	Electronic structure of indium oxide using cluster calculations. *Physical Review B*, **1997**, 56, 3536-3539	3.3	64
285	Atomic structures of supersaturated ZnO–Al2O3 solid solutions. *Journal of Applied Physics*, **2008**, 103, 014309	2.5	64
284	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	7.2	63
283	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
282	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
281	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

280	Sparse representation for a potential energy surface. *Physical Review B*, **2014**, 90,	3.3	59
279	Ionization potentials of (112) and (112□) facet surfaces of CuInSe2 and CuGaSe2. *Physical Review B*, **2012**, 86,	3.3	59
278	Comparison of approximations in density functional theory calculations: Energetics and structure of binary oxides. *Physical Review B*, **2017**, 96,	3.3	58
277	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
276	Evolution of crystal structures in metallic elements. *Physical Review B*, **2013**, 87,	3.3	56
275	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
274	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
273	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
272	Transition pathway of CO2 crystals under high pressures. *Physical Review B*, **2008**, 77,	3.3	54
271	Doping of hexagonal boron nitride via intercalation: A theoretical prediction. *Physical Review B*, **2010**, 81,	3.3	53
270	Near-edge x-ray-absorption fine structure of crystalline silicon dioxides. *Physical Review B*, **1995**, 52, 11733-11739	3.3	53
269	First-principles interatomic potentials for ten elemental metals via compressed sensing. *Physical Review B*, **2015**, 92,	3.3	52
268	First-principles study of native defects and lanthanum impurities in NaTaO3. *Physical Review B*, **2008**, 78,	3.3	52
267	Atomic structures and energetics of LaNi5H solid solution and hydrides. *Physical Review B*, **2001**, 64,	3.3	51
266	Impurity-Enhanced Intergranular Cavity Formation in Silicon Nitride at High Temperatures. *Journal of the American Ceramic Society*, **1991**, 74, 752-759	3.8	51
265	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
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263	Electronic and structural properties of the oxygen vacancy in BaTiO3. *Applied Physics Letters*, **2011**, 98, 172901	3.4	49

262	Prediction of the new spinel phase of Ti3N4 and SiTi2N4 and the metal-insulator transition. *Physical Review B*, **2000**, 61, 10609-10614	3.3	49
261	DynaPhoPy: A code for extracting phonon quasiparticles from molecular dynamics simulations. *Computer Physics Communications*, **2017**, 221, 221-234	4.2	48
260	First-principles multi-electron calculations for L(2,3) ELNES/XANES of 3d transition metal monoxides. *Ultramicroscopy*, **2006**, 106, 970-5	3.1	48
259	First-principles calculations of lattice dynamics in CdTiO3 and CaTiO3: Phase stability and ferroelectricity. *Physical Review B*, **2011**, 84,	3.3	47
258	First-Principles Calculations of Anion Vacancies in Oxides and Nitrides. *Journal of the American Ceramic Society*, **2004**, 85, 68-74	3.8	47
257	Local environment of Mn dopant in ZnO by near-edge x-ray absorption fine structure analysis. *Applied Physics Letters*, **2005**, 86, 121902	3.4	47
256	Electron energy loss near-edge structures of cubic Si3N4. *Applied Physics Letters*, **2001**, 78, 2134-2136	3.4	47
255	First principles study of dopant solubility and defect chemistry in LiCoO2. *Journal of Materials Chemistry A*, **2014**, 2, 11235-11245	13	46
254	Core-hole effect on dipolar and quadrupolar transitions of SrTiO3 and BaTiO3 at Ti K edge. *Physical Review B*, **2005**, 71,	3.3	46
253	Ab initio study of symmetric tilt boundaries in ZnO. *Physical Review B*, **2001**, 63,	3.3	46
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251	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
250	Band alignment of semiconductors and insulators using dielectric-dependent hybrid functionals: Toward high-throughput evaluation. *Physical Review B*, **2017**, 95,	3.3	45
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248	Defect chemistry of a BaZrO3 ⊟ (111) grain boundary by first principles calculations and space-charge theory. *Physical Chemistry Chemical Physics*, **2012**, 14, 12339-46	3.6	44
247	Tuning the chemical functionality of a gas sensitive material: Water adsorption on SnO2(1 0 1). *Surface Science*, **2006**, 600, 29-32	1.8	43
246	First-principles study of cation disordering in MgAl2O4 spinel with cluster expansion and Monte Carlo simulation. *Physical Review B*, **2006**, 73,	3.3	42
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243	Theoretical prediction of ELNES/XANES and chemical bondings of AlN polytypes. *Micron*, **2003**, 34, 249-54	2.3	40
242	Changes in Chemical Bondings by Li Deintercalation in LiMO2(M=Cr, V, Co and Ni). *Japanese Journal of Applied Physics*, **1999**, 38, 2024-2027	1.4	39
241	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
240	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
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238	Proton-Conducting Network in Lanthanum Orthophosphate. *Journal of Physical Chemistry C*, **2012**, 116, 19117-19124	3.8	38
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235	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
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233	Microstructure of Mn-doped □Ga2O3 epitaxial film on sapphire (0001) with room temperature ferromagnetism. *Journal of Applied Physics*, **2007**, 101, 063526	2.5	36
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231	First Principles Calculation of Defect Formation Energies in Sr- and Mg-Doped LaGaO3. *Journal of Physical Chemistry B*, **2004**, 108, 9168-9172	3.4	36
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228	Epitaxial growth of Mn-doped □Ga2O3 on spinel substrate. *Journal of Materials Research*, **2011**, 26, 578-583	2.3	35
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226	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
225	Atomistic Origin of Phase Stability in Oxygen-Functionalized MXene: A Comparative Study. *Journal of Physical Chemistry C*, **2017**, 121, 18947-18953	3.8	34
224	Atomic structure of luminescent centers in high-efficiency Ce-doped w-AlN single crystal. *Scientific Reports*, **2014**, 4, 3778	4.9	34
223	Effects of crystal structure on Co-L2,3 x-ray absorption near-edge structure and electron-energy-loss near-edge structure of trivalent cobalt oxides. *Physical Review B*, **2008**, 77,	3.3	34
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221	First-principles calculation on free energy of precipitate nucleation. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2004**, 28, 173-176	1.9	34
220	Functional complex point-defect structure in a huge-size-mismatch system. *Physical Review Letters*, **2013**, 110, 065504	7.4	33
219	Electronic structures of dynamically stable As2O3, Sb2O3, and Bi2O3 crystal polymorphs. *Physical Review B*, **2011**, 83,	3.3	33
218	First-principles-based phase diagram of the cubic BNC ternary system. *Physical Review B*, **2008**, 77,	3.3	33
217	Solubility of Si3N4 in Liquid SiO2. *Journal of the American Ceramic Society*, **2004**, 85, 25-32	3.8	33
216	Electron-energy-loss near edge structures of six-fold-coordinated Zn in MgO. *Ultramicroscopy*, **2001** , 86, 363-70	3.1	33
215	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
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209	Effective Doping in Cubic Si3N4 and Ge3N4: A First-Principles Study. *Journal of the American Ceramic Society*, **2004**, 85, 97-100	3.8	31

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203	Free-Energy Calculation of Precipitate Nucleation in an Fe-Cu-Ni Alloy. *Materials Transactions*, **2004**, 45, 1978-1981	1.3	28
202	Theoretical calculation for the multiplet structure of the tetrahedrally coordinated Cr4+ in Y3Al5O12. *Journal of Chemical Physics*, **2001**, 115, 492-508	3.9	28
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199	Strategy for managing both high strength and large ductility in structural materials□equential nucleation of different deformation modes based on a concept of plaston. *Scripta Materialia*, **2020**, 181, 35-42	5.6	27
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195	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
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193	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
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188	Processing and Mechanical Properties of Dense Si3N4-SiC-Whisker Composites without Sintering Aids. *Journal of the American Ceramic Society*, **1989**, 72, 1461-1464	3.8	25
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186	Proton trapping in Y and Sn Co-doped BaZrO3. *Journal of Materials Chemistry A*, **2015**, 3, 10045-10051	13	24
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