Isao Tanaka

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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	First principles phonon calculations in materials science. *Scripta Materialia*, **2015**, 108, 1-5	5.6	4076
411	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
410	High-density electron anions in a nanoporous single crystal: [Ca24Al28O64]4+(4e-). *Science*, **2003**, 301, 626-9	33.3	638
409	Distributions of phonon lifetimes in Brillouin zones. *Physical Review B*, **2015**, 91,	3.3	607
408	First-principles phonon calculations of thermal expansion in Ti3SiC2, Ti3AlC2, and Ti3GeC2. *Physical Review B*, **2010**, 81,	3.3	309
407	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
406	Band structure diagram paths based on crystallography. *Computational Materials Science*, **2017**, 128, 140-184	3.2	247
405	Phonon-phonon interactions in transition metals. *Physical Review B*, **2011**, 84,	3.3	235
404	Point defects in ZnO: an approach from first principles. *Science and Technology of Advanced Materials*, **2011**, 12, 034302	7.1	234
403	Lithium iron borates as high-capacity battery electrodes. *Advanced Materials*, **2010**, 22, 3583-7	24	204
402	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
401	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
400	Thermal physics of the lead chalcogenides PbS, PbSe, and PbTe from first principles. *Physical Review B*, **2014**, 89,	3.3	172
399	First-principles approach to chemical diffusion of lithium atoms in a graphite intercalation compound. *Physical Review B*, **2008**, 78,	3.3	160
398	Representation of compounds for machine-learning prediction of physical properties. *Physical Review B*, **2017**, 95,	3.3	158
397	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
396	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

395	First-principles study on lithium removal from Li2MnO3. *Journal of Power Sources*, **2009**, 189, 798-801	8.9	136
394	Discovery of earth-abundant nitride semiconductors by computational screening and high-pressure synthesis. *Nature Communications*, **2016**, 7, 11962	17.4	133
393	Pure H? conduction in oxyhydrides. *Science*, **2016**, 351, 1314-7	33.3	110
392	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
391	Soft longitudinal modes in spin-singlet CuGeO3. *Physical Review B*, **1994**, 50, 1278-1281	3.3	109
390	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
389	XANES and ELNES in Ceramic Science. *Journal of the American Ceramic Society*, **2005**, 88, 2013-2029	3.8	104
388	Design and synthesis of a magnesium alloy for room temperature hydrogen storage. *Acta Materialia*, **2018**, 149, 88-96	8.4	101
387	Decomposition reactions for NaAlH4, Na3AlH6, and NaH: First-principles study. *Physical Review B*, **2005**, 71,	3.3	93
386	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
385	Theoretical Formation Energy of Oxygen-Vacancies in Oxides. *Materials Transactions*, **2002**, 43, 1426-1429	1.3	91
384	Ab initio lattice dynamics and phase transformations of ZrO2. *Physical Review B*, **2005**, 71,	3.3	90
383	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
382	First-principles XANES simulations of spinel zinc ferrite with a disordered cation distribution. *Physical Review B*, **2007**, 75,	3.3	88
381	Raman-scattering study of CuGeO3 in the spin-Peierls phase. *Physical Review B*, **1994**, 50, 16468-16474	3.3	88
380	Accelerated discovery of cathode materials with prolonged cycle life for lithium-ion battery. *Nature Communications*, **2014**, 5, 4553	17.4	86
379	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
378	Theoretical Prediction of the Structure and Properties of Cubic Spinel Nitrides. *Journal of the American Ceramic Society*, **2004**, 85, 75-80	3.8	86

377	Reduced SnO2 surfaces by first-principles calculations. *Applied Physics Letters*, **2004**, 84, 909-911	3.4	85
376	Single crystal growth of superconducting La2-xSrxCuO4 by the TSFZ method. *Journal of Crystal Growth*, **1989**, 96, 711-715	1.6	85
375	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
374	Structural Analysis and Superconducting Properties of F-Substituted NdOBiS2 Single Crystals. *Journal of the Physical Society of Japan*, **2013**, 82, 113701	1.5	83
373	Complete elastic constants and giant softening of c66 in superconducting La1.86Sr0.14CuO4. *Physical Review Letters*, **1990**, 64, 2458-2461	7.4	77
372	Anti-ferrodistortive-like oxygen-octahedron rotation induced by the oxygen vacancy in cubic SrTiO3. *Advanced Materials*, **2013**, 25, 86-90	24	76
371	Unconventional lattice stiffening in superconducting La2-xSrxCuO4 single crystals. *Physical Review B*, **1995**, 52, 570-580	3.3	75
370	Growth and superconducting properties of F-substituted ROBiS2 (R=La, Ce, Nd) single crystals. *Solid State Communications*, **2014**, 178, 33-36	1.6	73
369	Temperature dependence of anisotropic lower critical fields in (La1-xSrx)2CuO4. *Physical Review B*, **1990**, 41, 4823-4826	3.3	73
368	Theoretical ELNES using one-particle and multi-particle calculations. *Micron*, **2010**, 41, 695-709	2.3	72
367	Identification of ultradilute dopants in ceramics. *Nature Materials*, **2003**, 2, 541-5	27	72
366	Lattice dynamics and thermodynamical properties of silicon nitride polymorphs. *Physical Review B*, **2008**, 78,	3.3	71
365	Crystal growth of Ca12Al14O33 by the floating zone method. *Journal of Crystal Growth*, **2002**, 237-239, 801-805	1.6	71
364	Interplay between lattice softening and high-Tc superconductivity in La1.86Sr0.14CuO4. *Physical Review Letters*, **1993**, 70, 3447-3450	7.4	67
363	Cubic and orthorhombic structures of aluminum hydride AlH3 predicted by a first-principles study. *Physical Review B*, **2005**, 71,	3.3	65
362	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	13	63
361	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
360	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

359	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
358	Sparse representation for a potential energy surface. *Physical Review B*, **2014**, 90,	3.3	59
357	Ionization potentials of (112) and (112̄) facet surfaces of CuInSe2 and CuGaSe2. *Physical Review B*, **2012**, 86,	3.3	59
356	Comparison of approximations in density functional theory calculations: Energetics and structure of binary oxides. *Physical Review B*, **2017**, 96,	3.3	58
355	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
354	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
353	Evolution of crystal structures in metallic elements. *Physical Review B*, **2013**, 87,	3.3	56
352	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
351	Crystal structures of LaO1−xFxBiS2 (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
350	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
349	Transition pathway of CO2 crystals under high pressures. *Physical Review B*, **2008**, 77,	3.3	54
348	First-principles interatomic potentials for ten elemental metals via compressed sensing. *Physical Review B*, **2015**, 92,	3.3	52
347	First-principles study of native defects and lanthanum impurities in NaTaO3. *Physical Review B*, **2008**, 78,	3.3	52
346	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
345	Electronic and structural properties of the oxygen vacancy in BaTiO3. *Applied Physics Letters*, **2011**, 98, 172901	3.4	49
344	Superconducting double perovskite bismuth oxide prepared by a low-temperature hydrothermal reaction. *Angewandte Chemie - International Edition*, **2014**, 53, 3599-603	16.4	48
343	DynaPhoPy: A code for extracting phonon quasiparticles from molecular dynamics simulations. *Computer Physics Communications*, **2017**, 221, 221-234	4.2	48
342	First-Principles Calculations of Anion Vacancies in Oxides and Nitrides. *Journal of the American Ceramic Society*, **2004**, 85, 68-74	3.8	47

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340	Core-hole effect on dipolar and quadrupolar transitions of SrTiO3 and BaTiO3 at Ti K edge. *Physical Review B*, **2005**, 71,	3.3	46
339	Thermal contraction at the spin-Peierls transition in CuGeO3. *Physical Review B*, **1994**, 50, 12606-12610	3.3	46
338	Relation between structure and doping in La2SrxCuO4+ a neutron diffraction study on single crystals. *Physica C: Superconductivity and Its Applications*, **1994**, 223, 396-416	1.3	46
337	Inversion symmetry breaking by oxygen octahedral rotations in the Ruddlesden-Popper NaRTiO4 family. *Physical Review Letters*, **2014**, 112, 187602	7.4	45
336	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
335	Band alignment of semiconductors and insulators using dielectric-dependent hybrid functionals: Toward high-throughput evaluation. *Physical Review B*, **2017**, 95,	3.3	45
334	Synthesis and electrochemistry of monoclinic Li(MnxFe1)BO3: a combined experimental and computational study. *Journal of Materials Chemistry*, **2011**, 21, 10690		45
333	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
332	Defect chemistry of a BaZrO3 3 (111) grain boundary by first principles calculations and space-charge theory. *Physical Chemistry Chemical Physics*, **2012**, 14, 12339-46	3.6	44
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330	Impact of Chemical Fluctuations on Stacking Fault Energies of CrCoNi and CrMnFeCoNi High Entropy Alloys from First Principles. *Entropy*, **2018**, 20,	2.8	42
329	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
328	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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323	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
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321	Oxygen vacancy formation and reduction properties of β-MnO2 grain boundaries and the potential for high electrochemical performance. *ACS Applied Materials & Interfaces*, **2014**, 6, 17776-84	9.5	36
320	Theoretical Study on the Chemistry of Intergranular Glassy Film in Si3N4–SiO2 Ceramics. *Journal of the American Ceramic Society*, **2004**, 85, 109-112	3.8	36
319	Geometric ferroelectricity in rare-earth compounds RGaO3 and RInO3. *Physical Review B*, **2009**, 79,	3.3	36
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317	Epitaxial growth of Mn-doped β-Ga2O3 on spinel substrate. *Journal of Materials Research*, **2011**, 26, 578-583	2.5	35
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315	Electronic States of Sulfur Doped TiO2 by First Principles Calculations. *Materials Transactions*, **2004**, 45, 1987-1990	1.3	35
314	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
313	Atomistic Origin of Phase Stability in Oxygen-Functionalized MXene: A Comparative Study. *Journal of Physical Chemistry C*, **2017**, 121, 18947-18953	3.8	34
312	Atomic structure of luminescent centers in high-efficiency Ce-doped w-AlN single crystal. *Scientific Reports*, **2014**, 4, 3778	4.9	34
311	Functional complex point-defect structure in a huge-size-mismatch system. *Physical Review Letters*, **2013**, 110, 065504	7.4	33
310	Electronic structures of dynamically stable As2O3, Sb2O3, and Bi2O3 crystal polymorphs. *Physical Review B*, **2011**, 83,	3.3	33
309	First-principles-based phase diagram of the cubic BNC ternary system. *Physical Review B*, **2008**, 77,	3.3	33
308	Solubility of Si3N4 in Liquid SiO2. *Journal of the American Ceramic Society*, **2004**, 85, 25-32	3.8	33
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306	Categorization of surface polarity from a crystallographic approach. *Computational Materials Science*, **2016**, 113, 221-230	3.2	31

305	Proximity to Fermi-surface topological change in superconducting LaO0.54F0.46BiS2. *Physical Review B*, **2014**, 90,	3.3	31
304	Theoretical Photovoltaic Conversion Efficiencies of ZnSnP2, CdSnP2, and Zn1-xCdxSnP2Alloys. *Applied Physics Express*, **2013**, 6, 061201	2.4	31
303	Effective Doping in Cubic Si3N4 and Ge3N4: A First-Principles Study. *Journal of the American Ceramic Society*, **2004**, 85, 97-100	3.8	31
302	Characterization and structural analysis of twinned La2−xSrxCuO4±δ crystals by neutron diffraction. *Physica C: Superconductivity and Its Applications*, **1992**, 191, 455-468	1.3	31
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300	Structure, Superconductivity, and Magnetism of Ce(O,F)BiS2 Single Crystals. *Crystal Growth and Design*, **2015**, 15, 39-44	3.5	29
299	Direct evidence of hidden local spin polarization in a centrosymmetric superconductor LaO FBiS. *Nature Communications*, **2017**, 8, 1919	17.4	29
298	Phonon softening in paramagnetic bcc Fe and its relationship to the pressure-induced phase transition. *Physical Review B*, **2014**, 90,	3.3	29
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294	Strong Spin-Lattice Coupling Through Oxygen Octahedral Rotation in Divalent Europium Perovskites. *Advanced Functional Materials*, **2013**, 23, 1864-1872	15.6	28
293	Free-Energy Calculation of Precipitate Nucleation in an Fe-Cu-Ni Alloy. *Materials Transactions*, **2004**, 45, 1978-1981	1.3	28
292	Coexistence of superconductivity and charge-density wave in the quasi-one-dimensional material HfTe. *Scientific Reports*, **2017**, 7, 45217	4.9	27
291	Classification of spinel structures based on first-principles cluster expansion analysis. *Physical Review B*, **2010**, 81,	3.3	27
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289	Evaluation of Migration Energy of Lithium Ions in Chalcogenides and Halides by First Principles Calculation. *Materials Transactions*, **2002**, 43, 1460-1463	1.3	26
288	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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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	Proton trapping in Y and Sn Co-doped BaZrO3. *Journal of Materials Chemistry A*, **2015**, 3, 10045-10051	13	24
284	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
283	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
282	Mode decomposition based on crystallographic symmetry in the band-unfolding method. *Physical Review B*, **2017**, 95,	3.3	23
281	Theoretical Prediction of Post-Spinel Phases of Silicon Nitride. *Journal of the American Ceramic Society*, **2004**, 85, 7-10	3.8	23
280	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
279	Elastic and inelastic neutron scattering studies on the tetragonal to orthorhombic phase transition of La2 Sr x CuO4 *European Physical Journal B*, **1994**, 94, 29-37	1.2	23
278	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
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276	Compositional descriptor-based recommender system for the materials discovery. *Journal of Chemical Physics*, **2018**, 148, 241719	3.9	22
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273	Atomistic mechanism of proton conduction in solid CsHSO4 by a first-principles study. *Physical Review B*, **2004**, 69,	3.3	22
272	Valence state of Ti in conductive nanowires in sapphire. *Physical Review B*, **2004**, 70,	3.3	22
271	Local Chemical Bonding around Rare-Earth Ions in - and Si3N4. *Journal of the American Ceramic Society*, **2005**, 80, 2525-2532	3.8	22
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269	Electronic insulator-conductor conversion in hydride ion-doped 12CaO·7Al2O3 by electron-beam irradiation. *Applied Physics Letters*, **2005**, 86, 022109	3.4	21
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265	C-axis electrical resistivity of PrO1−xFaBiS2single crystals. *Japanese Journal of Applied Physics*, **2015**, 54, 083101	1.4	20
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263	Tetravalent dysprosium in a perovskite-type oxide. *Advanced Materials*, **2012**, 24, 2051-3	24	20
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256	Formation energy of Cr/Al vacancies in spinel MgCr2O4 and MgAl2O4 by first-principles calculations. *Physical Review B*, **2002**, 65,	3.3	19
255	Electronic Mechanism of Ag-Cluster Formation in AgBr and AgI. *Journal of the Physical Society of Japan*, **1998**, 67, 2027-2036	1.5	19
254	Electronic Structure and Defect Chemistry of Tin(II) Complex Oxide SnNb2O6. *Journal of Physical Chemistry C*, **2016**, 120, 9604-9611	3.8	19
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250	Effects of tilting mirrors on the solid□quid interface during floating zone growth using tilting-mirror-type infrared-heating image furnace. *Journal of Crystal Growth*, **2010**, 312, 2008-2011	1.6	18
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244	Proton incorporation and trapping in ZrO2 grain boundaries. *Journal of Materials Chemistry A*, **2014**, 2, 1400-1408	13	17
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