Atsushi Togo

List of Publications by Year in Descending Order

40 papers	11,225 citations	26 h-index	42 g-index
42 ext. papers	13,955 ext. citations	4 avg, IF	7.12 L-index

#	Paper	IF	Citations
40	Collective Motion of Atoms in Metals by First Principles Calculations **2022**, 79-90		
39	Group-theoretical high-order rotational invariants for structural representations: Application to linearized machine learning interatomic potential. *Physical Review B*, **2019**, 99,	3.3	19
38	Finite-displacement computation of the electron-phonon interaction within the projector augmented-wave method. *Physical Review B*, **2019**, 100,	3.3	6
37	Descriptors for Machine Learning of Materials Data **2018**, 3-23		26
36	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
35	Provenance, workflows, and crystallographic tools in materials science: AiiDA, spglib, and seekpath. *MRS Bulletin*, **2018**, 43, 696-702	3.2	4
34	Mode decomposition based on crystallographic symmetry in the band-unfolding method. *Physical Review B*, **2017**, 95,	3.3	23
33	DynaPhoPy: A code for extracting phonon quasiparticles from molecular dynamics simulations. *Computer Physics Communications*, **2017**, 221, 221-234	4.2	48
32	Anharmonicity in the High-Temperature Cmcm Phase of SnSe: Soft Modes and Three-Phonon Interactions. *Physical Review Letters*, **2016**, 117, 075502	7.4	104
31	Low phonon conductivity of layered BiCuOS, BiCuOSe, and BiCuOTe from first principles. *Physical Review B*, **2016**, 94,	3.3	17
30	Suppression of lattice thermal conductivity by mass-conserving cation mutation in multi-component semiconductors. *APL Materials*, **2016**, 4, 104809	5.7	8
29	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
28	Distributions of phonon lifetimes in Brillouin zones. *Physical Review B*, **2015**, 91,	3.3	607
27	First principles phonon calculations in materials science. *Scripta Materialia*, **2015**, 108, 1-5	5.6	4076
26	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
25	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
24	First principles study of thermal conductivity cross-over in nanostructured zinc-chalcogenides. *Journal of Applied Physics*, **2015**, 117, 045102	2.5	20

23	Inversion symmetry breaking by oxygen octahedral rotations in the Ruddlesden-Popper NaRTiO4 family. *Physical Review Letters*, **2014**, 112, 187602	7.4	45
22	Ab initio ORTEP drawings: a case study of N-based molecular crystals with different chemical nature. *CrystEngComm*, **2014**, 16, 10907-10915	3.3	28
21	Phonon softening in paramagnetic bcc Fe and its relationship to the pressure-induced phase transition. *Physical Review B*, **2014**, 90,	3.3	29
20	Thermal physics of the lead chalcogenides PbS, PbSe, and PbTe from first principles. *Physical Review B*, **2014**, 89,	3.3	172
19	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
18	Evolution of crystal structures in metallic elements. *Physical Review B*, **2013**, 87,	3.3	56
17	First-order Raman scattering of the MAX phases: Ti2AlN, Ti2AlC0.5N0.5, Ti2AlC, (Ti0.5V0.5)2AlC, V2AlC, Ti3AlC2, and Ti3GeC2. *Journal of Raman Spectroscopy*, **2012**, 43, 168-172	2.3	109
16	Neutron diffraction measurements and first-principles study of thermal motion of atoms in select Mn+1AXn and binary MX transition-metal carbide phases. *Physical Review B*, **2012**, 86,	3.3	30
15	Point defects in ZnO: an approach from first principles. *Science and Technology of Advanced Materials*, **2011**, 12, 034302	7.1	234
14	Electronic structures of dynamically stable As2O3, Sb2O3, and Bi2O3 crystal polymorphs. *Physical Review B*, **2011**, 83,	3.3	33
13	Phonon-phonon interactions in transition metals. *Physical Review B*, **2011**, 84,	3.3	235
12	Doping of hexagonal boron nitride via intercalation: A theoretical prediction. *Physical Review B*, **2010**, 81,	3.3	53
11	First-principles phonon calculations of thermal expansion in Ti3SiC2, Ti3AlC2, and Ti3GeC2. *Physical Review B*, **2010**, 81,	3.3	309
10	Anisotropic phonon density of states in FePt nanoparticles with L10 structure. *Physical Review B*, **2010**, 81,	3.3	9
9	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
8	Thermodynamics and structures of oxide crystals by a systematic set of first principles calculations. *Journal of Materials Chemistry*, **2010**, 20, 10335		7
7	Native defects in oxide semiconductors: a density functional approach. *Journal of Physics Condensed Matter*, **2010**, 22, 384211	1.8	41
6	Defect energetics in ZnO: A hybrid Hartree-Fock density functional study. *Physical Review B*, **2008**, 77,	3.3	613

5	Structure and stability of a homologous series of tin oxides. *Physical Review Letters*, **2008**, 100, 045702	7.4	129
4	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
3	Transition pathway of CO2 crystals under high pressures. *Physical Review B*, **2008**, 77,	3.3	54
2	First-principles lattice dynamics calculations of the phase boundary between beta-Si3N4 and gamma-Si3N4 at elevated temperatures and pressures. *Journal of Computational Chemistry*, **2008**, 29, 2255-9	3.5	27
1	Poster: Electronic Structure, Lattice Dynamics, and Transport471-522		