Atsushi Togo

List of Publications by Year
in descending order

40 papers	16,587 citations	186209 28 h-index	302012 39 g-index
42 all docs	42 docs citations	42 times ranked	14126 citing authors

#	Article	IF	Citations
1	First principles phonon calculations in materials science. Scripta Materialia, 2015, 108, 1-5.	2.6	7,324
2	First-principles calculations of the ferroelastic transition between rutile-type and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CaCl</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu high pressures. Physical Review B, 2008, 78, .	1.1	4,498
3	Distributions of phonon lifetimes in Brillouin zones. Physical Review B, 2015, 91, .	1.1	963
4	Defect energetics in ZnO: A hybrid Hartree-Fock density functional study. Physical Review B, 2008, 77, .	1.1	655
5	First-principles phonon calculations of thermal expansion in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ti</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ti</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub Physical Review B, 2010, 81, .	1.1	429
6	Phonon-phonon interactions in transition metals. Physical Review B, 2011, 84, .	1.1	363
7	Prediction of Low-Thermal-Conductivity Compounds with First-Principles Anharmonic Lattice-Dynamics Calculations and Bayesian Optimization. Physical Review Letters, 2015, 115, 205901.	2.9	343
8	Point defects in ZnO: an approach from first principles. Science and Technology of Advanced Materials, 2011, 12, 034302.	2.8	279
9	Thermal physics of the lead chalcogenides PbS, PbSe, and PbTe from first principles. Physical Review B, 2014, 89, .	1.1	212
10	First-order Raman scattering of the MAX phases: Ti₂AlN, Ti₂AlC_{0.5}N_{0.5}, Ti₂AlC, (Ti_{0.5}V_{0.5})₂AlC, V₂AlC, Ti₃AlC₂, and Ti₃GeC₂. Journal of Raman Spectroscopy, 2012, 43, 168-172.	1.2	159
11	Anharmonicity in the High-Temperature <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>C</mml:mi><mml:mi>m</mml:mi><mml:mi>c</mml:mi><mml:mi>m</mml:mi></mml:math> Phase of SnSe: Soft Modes and Three-Phonon Interactions. Physical Review Letters, 2016, 117, 075502.	2.9	247
12	Structure and Stability of a Homologous Series of Tin Oxides. Physical Review Letters, 2008, 100, 045702.	2.9	146
13	DynaPhoPy: A code for extracting phonon quasiparticles from molecular dynamics simulations. Computer Physics Communications, 2017, 221, 221-234.	3.0	105
14	Influence of the exchange-correlation functional on the quasi-harmonic lattice dynamics of II-VI semiconductors. Journal of Chemical Physics, 2015, 143, 064710.	1.2	80
15	Evolution of crystal structures in metallic elements. Physical Review B, 2013, 87, .	1.1	78
16	High-pressure torsion of titanium at cryogenic and room temperatures: Grain size effect on allotropic phase transformations. Acta Materialia, 2014, 68, 207-213.	3.8	78
17	Transition pathway of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> crystals under high pressures. Physical Review B, 2008, 77, .	1.1	65
18	Lattice thermal conductivities of two <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mm polymorphs by first-principles calculations and the phonon Boltzmann transport equation. Physical Review B, 2018, 97, .	1.1	65

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19	Doping of hexagonal boron nitride via intercalation: A theoretical prediction. Physical Review B, 2010, 81, .	1.1	61
20	Inversion Symmetry Breaking by Oxygen Octahedral Rotations in the Ruddlesden-Popper<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Na</mml:mi><mml:mi>R</mml:mi><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mr Physical Review Letters, 2014, 112, 187602.	2.9	60
21	Native defects in oxide semiconductors: a density functional approach. Journal of Physics Condensed Matter, 2010, 22, 384211.	0.7	47
22	Mode decomposition based on crystallographic symmetry in the band-unfolding method. Physical Review B, 2017, 95, .	1.1	46
23	Descriptors for Machine Learning of Materials Data. , 2018, , 3-23.		45
24	Electronic structures of dynamically stable As<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Neutron diffraction measurements and first principles study of thermal motion of atoms in	1.1	38
25	selected binary<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>M</mml:mi><mml:mrow><mml:mi>n</mml:mi><mml:mo>+</mml:mo></mml:mr binary<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>M</mml:mi><mml:mi>X</mml:mi> Physical Review B, 2012, 86, .	1.1	38
26	Phonon softening in paramagnetic bcc Fe and its relationship to the pressure-induced phase transition. Physical Review B, 2014, 90, .	1.1	36
27	Ab initio ORTEP drawings: a case study of N-based molecular crystals with different chemical nature. CrystEngComm, 2014, 16, 10907-10915.	1.3	32
28	Group-theoretical high-order rotational invariants for structural representations: Application to linearized machine learning interatomic potential. Physical Review B, 2019, 99, .	1.1	31
29	Firstâ€principles lattice dynamics calculations of the phase boundary between Î²â€Si₃N₄ and Î³â€Si₃N₄ at elevated temperatures and pressures. Journal of Computational Chemistry, 2008, 29, 2255-2259.	1.5	28
30	Improper Inversion Symmetry Breaking and Piezoelectricity through Oxygen Octahedral Rotations in Layered Perovskite Family, LiRTiO₄ (R = Rare Earths). Advanced Electronic Materials, 2016, 2, 1500196.	2.6	28
31	Low phonon conductivity of layered BiCuOS, BiCuOSe, and BiCuOTe from first principles. Physical Review B, 2016, 94, .	1.1	28
32	First principles study of thermal conductivity cross-over in nanostructured zinc-chalcogenides. Journal of Applied Physics, 2015, 117, .	1.1	23
33	Finite-displacement computation of the electron-phonon interaction within the projector augmented-wave method. Physical Review B, 2019, 100, .	1.1	14
34	Suppression of lattice thermal conductivity by mass-conserving cation mutation in multi-component semiconductors. APL Materials, 2016, 4, 104809.	2.2	12
35	Anisotropic phonon density of states in FePt nanoparticles withL10structure. Physical Review B, 2010, 81, .	1.1	9
36	Thermodynamics and structures of oxide crystals by a systematic set of first principles calculations. Journal of Materials Chemistry, 2010, 20, 10335.	6.7	7

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37	Provenance, workflows, and crystallographic tools in materials science: AiiDA, spglib, and seekpath. MRS Bulletin, 2018, 43, 696-702.	1.7	6
38	LO-mode phonon of KCl and NaCl at 300â€‰K by inelastic x-ray scattering measurements and first principles calculations. Journal of Physics Condensed Matter, 2022, 34, 365401.	0.7	6
39	Phonon structure of titanium under shear deformation along <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>{</mml:mo><mml:mn>10</mml:mn><mml:mover accent="true"><mml:mn>1</mml:mn><mml:mo>Â¯</mml:mo></mml:mover><mml:mn>2</mml:mn><mml:mo>}</mml:mo></mml:mro twinning mode. Physical Review B, 2020, 102, .	1.1	2
40	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.	0.7	1