Toshiaki Iitaka

List of Publications by Year
in descending order

92	2,796	185998 28	182168 51
papers	citations	h-index	g-index

94	94	94	2367
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Superconductive sodalite-like clathrate calcium hydride at high pressures. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 6463-6466.	3.3	630
2	Superconducting High Pressure Phase of Germane. Physical Review Letters, 2008, 101, 107002.	2.9	224
3	High-pressure crystal structures and superconductivity of Stannane (SnH ₄). Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 1317-1320.	3.3	168
4	Dissociation of methane under high pressure. Journal of Chemical Physics, 2010, 133, 144508.	1.2	101
5	Design and performance of high-pressure PLANET beamline at pulsed neutron source at J-PARC. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2015, 780, 55-67.	0.7	96
6	Computational discovery of a dynamically stable cubic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SH</mml:mi><mml:mn>3</mml:mn></mml:msub></mml: -like high-temperature superconductor at 100ÂGPa via <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CH</mml:mi><mml:mn>4</mml:mn></mml:msub></mml intercalation. Physical Review B, 2020, 101, .	1.1	73
7	Compression of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>H</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:mtext>O</mml:m to 126 GPa and implications for hydrogen-bond symmetrization: Synchrotron x-ray diffraction measurements and density-functional calculations. Physical Review B, 2008, 77, .	1.1	72
8	Calculating the linear response functions of noninteracting electrons with a time-dependent SchrÃ¶dinger equation. Physical Review E, 1997, 56, 1222-1229.	0.8	68
9	Random phase vector for calculating the trace of a large matrix. Physical Review E, 2004, 69, 057701.	0.8	68
10	Solving the time-dependent SchrÃ¶dinger equation numerically. Physical Review E, 1994, 49, 4684-4690.	0.8	66
11	Failure of Conventional Density Functionals for the Prediction of Molecular Crystal Polymorphism: A Quantum Monte Carlo Study. Journal of Physical Chemistry Letters, 2010, 1, 1789-1794.	2.1	61
12	First-principles calculation of elastic properties of solid argon at high pressures. Physical Review B, 2001, 65, .	1.1	52
13	Enhancement of entanglement transfer in a spin chain by phase-shift control. Physical Review A, 2007, 75, .	1.0	50
14	Metallization and superconductivity of BeH2 under high pressure. Journal of Chemical Physics, 2014, 140, 124707.	1.2	50
15	First-principles calculation of helical spin order in iron perovskite SrFeO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>and BaFeO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 85, .	1.1	47
16	Algorithm for Linear Response Functions at Finite Temperatures: Application to ESR Spectrum ofs=12Antiferromagnet Cu Benzoate. Physical Review Letters, 2003, 90, 047203.	2.9	46
17	First-Principles Prediction on the High-Pressure Structures of Transition Metal Diborides (TMB₂, TM = Sc, Ti, Y, Zr). Inorganic Chemistry, 2010, 49, 6859-6864.	1.9	41
18	Poirierite, a dense metastable polymorph of magnesium iron silicate in shocked meteorites. Communications Earth & Environment, 2021, 2, .	2.6	41

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19	Structural morphologies of high-pressure polymorphs of strontium hydrides. Physical Chemistry Chemical Physics, 2015, 17, 19379-19385.	1.3	39
20	Methane hydrate under high pressure. Physical Review B, 2003, 68, .	1.1	37
21	Second-harmonic generation in noncentrosymmetric phosphates. Physical Review B, 2017, 96, .	1.1	37
22	Pressure-induced ferromagnetism in cubic perovskite SrFeO3and BaFeO3. Physical Review B, 2012, 86, .	1.1	35
23	HgTe: A potential thermoelectric material in the cinnabar phase. Journal of Chemical Physics, 2008, 128, 194713.	1.2	33
24	Prediction of Above-Room-Temperature Superconductivity in Lanthanide/Actinide Extreme Superhydrides. Journal of the American Chemical Society, 2022, 144, 13394-13400.	6.6	33
25	Electrical conductivity of ice VII. Scientific Reports, 2014, 4, 5778.	1.6	32
26	Second harmonic generation in the Weyl semimetal TaAs from a quantum kinetic equation. Physical Review B, 2018, 97, .	1.1	32
27	First-principles study of liquid gallium at ambient and high pressure. Journal of Chemical Physics, 2011, 135, 044507.	1.2	28
28	Stabilization of H3+ in the high pressure crystalline structure of HnCl (n = 2â€“7). Chemical Science, 2015, 6, 522-526.	3.7	28
29	Nonlinear electronic polarization and optical response in borophosphate<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BPO</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math> Physical Review B, 2016, 93, .	1.1	28
30	Linear scaling calculation for optical-absorption spectra of large hydrogenated silicon nanocrystallites. Physical Review B, 1997, 56, R4348-R4350.	1.1	27
31	Diffusion Monte Carlo Study of Para-Diiodobenzene Polymorphism Revisited. Journal of Chemical Theory and Computation, 2015, 11, 907-917.	2.3	22
32	Quantum-size effect in model nanocrystalline/amorphous mixed-phase silicon structures. Physical Review B, 1999, 59, 10309-10314.	1.1	21
33	Enhanced thermionic emission performance of LaB6 by Ce doping. Journal of Alloys and Compounds, 2018, 760, 1-5.	2.8	21
34	Electron density topology of high-pressure<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Ba</mml:mi><mml:mn>8</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">Si</mml:mi><mml:mn>46</mml:mn></mml:msub></mml:mrow></mml:math>from a combined Rietveld and maximum-entropy analysis. Physical Review B, 2007, 76, .	1.1	20
35	First principles molecular dynamics study of filled ice hydrogen hydrate. Journal of Chemical Physics, 2012, 137, 084505.	1.2	19
36	Raman and x-ray diffraction studies of Ba doped germanium clathrate Ba8Ge43 at high pressures. Journal of Applied Physics, 2007, 101, 063549.	1.1	18

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37	Pressure-Induced Intermolecular Interactions in Crystalline Silane-Hydrogen. Physical Review Letters, 2010, 105, 215501.	2.9	18
38	Pressure-induced isostructural phase transition of metal-doped silicon clathrates. Physical Review B, 2007, 75, .	1.1	17
39	Hydrogen segregation and its roles in structural stability and metallization: silane under pressure. Scientific Reports, 2015, 5, 13039.	1.6	17
40	Structural dynamics of basaltic melt at mantle conditions with implications for magma oceans and superplumes. Nature Communications, 2020, 11, 4815.	5.8	17
41	First-principles investigation on the geometry and electronic structure of the three-dimensional cuboidal C60 polymer. Journal of Chemical Physics, 2007, 127, 134906.	1.2	16
42	High pressure polyhydrides of molybdenum: A first-principles study. Solid State Communications, 2016, 239, 14-19.	0.9	15
43	GdN thin film: Chern insulating state on square lattice. Physical Review B, 2015, 92, .	1.1	14
44	Predicted Weyl fermions in magnetic GdBi and GdSb. International Journal of Modern Physics B, 2017, 31, 1750217.	1.0	13
45	Optical response of the chiral topological semimetal RhSi. Physical Review B, 2019, 100, .	1.1	13
46	Temperature Dependence of ESR Intensity for the Nanoscale Molecular Magnet V15. Journal of the Physical Society of Japan, 2005, 74, 107-110.	0.7	12
47	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>NaPN</mml:mi><mml:mn>2</mml:mn></mml:msub><m : Deep-ultraviolet nonlinear optical material with unprecedented strong second-harmonic generation coefficient. Physical Review Materials, 2019, 3, .	0.9	11
48	First-Principles Pseudo-Potential Study of the Pd(110)-c(2Ã—2)-Ethylene Adsorption System. Journal of Physical Chemistry B, 2001, 105, 8149-8154.	1.2	9
49	First-principles studies of liquid lithium under pressure. Journal of Physics Condensed Matter, 2010, 22, 095503.	0.7	9
50	Pressure-induced dissociation of water molecules in ice VII. Scientific Reports, 2015, 5, 12551.	1.6	9
51	Exploration of stable stoichiometries, physical properties and hardness in the Rhâ€“Si system: a first-principles study. RSC Advances, 2015, 5, 53497-53503.	1.7	9
52	The first peak splitting of the GeGe pair RDF in the correlation to network structure of GeO2 under compression. Journal of Non-Crystalline Solids, 2017, 459, 103-110.	1.5	9
53	Structures and Stability of Iron Halides at the Earthâ€™s Mantle and Core Pressures: Implications for the Missing Halogen Paradox. ACS Earth and Space Chemistry, 2018, 2, 711-719.	1.2	8
54	First-principles calculations of the epsilon phase of solid oxygen. Scientific Reports, 2019, 9, 8731.	1.6	8

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55	Crystallization of amorphous silica under compression. Canadian Journal of Physics, 2019, 97, 1133-1139.	0.4	8
56	ESR intensity and the Dzyaloshinsky-Moriya interaction of the nanoscale molecular magnet V<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>15</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 86, .	1.1	7
57	A Benchmark Quantum Monte Carlo Study of Molecular Crystal Polymorphism: A Challenging Case for Density-Functional Theory. ACS Symposium Series, 2012, , 101-117.	0.5	7
58	Simulating Proton Dynamics in High-Pressure Ice. Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu, 2013, 23, 124-132.	0.1	7
59	Calculating response functions in time domain with nonorthonormal basis sets. Physical Review E, 2000, 61, R3314-R3317.	0.8	6
60	Structural organization, micro-phase separation and polyamorphism of liquid MgSiO3 under compression. European Physical Journal B, 2016, 89, 1.	0.6	6
61	Computer simulation of CaSiO₃glass under compression: correlation between Siâ€“Si pair radial distribution function and intermediate range order structure. Materials Research Express, 2017, 4, 065201.	0.8	6
62	Optical detection of quantum geometric tensor in intrinsic semiconductors. Science China: Physics, Mechanics and Astronomy, 2021, 64, 1.	2.0	6
63	Stability of the symmetric multistep methods for the time-dependent SchrÃ¶dinger equation. Computer Physics Communications, 1995, 90, 251-259.	3.0	5
64	Efficient algorithm for calculating two-photon absorption spectra. Physical Review E, 1999, 60, R1178-R1180.	0.8	5
65	Dynamics of elemental lithium at megabar pressures. Physical Review B, 2006, 73, .	1.1	5
66	A method for calculating the eigenvalues of large Hermitian matrices by second-order recursion formulae. Computer Physics Communications, 1996, 96, 217-231.	3.0	4
67	Correlation functions for a time-dependent calculation of linear-response functions. Physical Review E, 1997, 56, 7318-7319.	0.8	4
68	ELECTRONIC AND MAGNETIC STRUCTURE OF THE HIGH PRESSURE PHASE OF Li₂CuO₂. International Journal of Modern Physics B, 2011, 25, 3409-3414.	1.0	4
69	Topology of SiO_x-units and glassy network of magnesium silicate glass under densification: correlation between radial distribution function and bond angle distribution. Modelling and Simulation in Materials Science and Engineering, 2020, 28, 065007.	0.8	4
70	Filled ice structure of gas hydratesâ€”a density functional study. Journal of Physics Condensed Matter, 2004, 16, S1171-S1176.	0.7	3
71	Electronic structure of dense solid oxygen from insulator to metal investigated with X-ray Raman scattering. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 21385-21391.	3.3	3
72	Crystal structures and superconductivity of carbonaceous sulfur hydrides at pressures up to 300 GPa. Physical Review B, 2022, 105, .	1.1	3

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73	Computational quantum dynamics in atomic physics. Nuclear Instruments & Methods in Physics Research B, 1995, 96, 663-667.	0.6	2
74	Non-degenerate two photon absorption spectra of Si nanocrystallites. Microelectronic Engineering, 1999, 47, 321-323.	1.1	2
75	Band topologies of hexaborides CaB6 and EuB6. Science China: Physics, Mechanics and Astronomy, 2017, 60, 1.	2.0	2
76	Two-domain structure and dynamics heterogeneity in a liquid SiO2. Journal of Non-Crystalline Solids, 2018, 484, 124-131.	1.5	2
77	Preparation and Properties of Highâ€Quality Ce_xLa_yPr_yNd_{0.05}Gd_{0.05}B₆ Single Crystal by Optical Floatâ€Zone Technique. Physica Status Solidi (A) Applications and Materials Science, 2019, 216, 1800706.	0.8	2
78	Berry curvature induced linear electro-optic effect in chiral topological semimetals. Physical Review B, 2022, 105, .	1.1	2
79	Focusing of tunneling electron in a magnetic field. Surface Science, 1999, 441, 283-288.	0.8	1
80	Terahertz nonlinear optics of chiral semimetals RhSn, HfSn, and PdGa. European Physical Journal B, 2021, 94, 1.	0.6	1
81	Interaction of Fast Neutral Atom and Surface. Journal of the Physical Society of Japan, 1989, 58, 445-450.	0.7	0
82	Phase Breaking in a Quantum Billiard. International Journal of Bifurcation and Chaos in Applied Sciences and Engineering, 1997, 07, 937-943.	0.7	0
83	Calculating the density of states and the linear response functions with time-dependent Schroedinger equations. Microelectronic Engineering, 1998, 43-44, 459-470.	1.1	0
84	Calculating Feynman Diagrams in Time Domain. Progress of Theoretical Physics Supplement, 2000, 138, 66-71.	0.2	0
85	ESR Intensity and Anisotropy of the Nanoscale Molecular Magnet V15. AIP Conference Proceedings, 2006, , .	0.3	0
86	Linear scaling calculation of ann-type GaAs quantum dot. Physical Review E, 2007, 76, 037701.	0.8	0
87	Large scale simulation of quantum-mechanical molecular dynamics for nano-polycrystalline diamond. Journal of Physics: Conference Series, 2010, 215, 012118.	0.3	0
88	GPU-accelerated large-scale quantum molecular dynamics simulation of 3-dimensional C₆₀polymers. Journal of Physics: Conference Series, 2010, 215, 012119.	0.3	0
89	Structures and Properties of Materials in the Deep Earth and Planets. Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu, 2017, 27, 174-182.	0.1	0
90	Simulation of structural characteristics of Mullite melt at high pressure. International Journal of Modern Physics B, 2018, 32, 1850271.	1.0	0

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91	Exotic high-pressure behavior of double nitride CuPN2. Computational Materials Science, 2018, 152, 217-222.	1.4	0
92	Optical-field induced SU(2) pair potential in caesium lead halide perovskites. International Journal of Modern Physics B, 2021, 35, 2150030.	1.0	0