Mayanak Kumar Gupta

List of Publications by Year
in descending order

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84 papers	1,098 citations	471371 17 h-index	477173 29 g-index
98 all docs	98 docs citations	98 times ranked	1382 citing authors

#	Article	IF	Citations
1	Phonons and anomalous thermal expansion behaviour in crystalline solids. Progress in Materials Science, 2018, 92, 360-445.	16.0	116
2	Inelastic neutron scattering and lattice dynamics of minerals. European Journal of Mineralogy, 2002, 14, 291-329.	0.4	76
3	Ab initio lattice dynamics simulations and inelastic neutron scattering spectra for studying phonons in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BaFe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> Effect of structural phase transition, structural relaxation, and magnetic ordering. Physical Review B, 2009, 79, .	1.1	64
4	Structural and electrical properties of layered perovskite type Pr₂Ti₂O₇: experimental and theoretical investigations. Journal of Materials Chemistry C, 2015, 3, 4570-4584.	2.7	45
5	Negative thermal expansion in cubic ZrW<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow />	1.1	44
6	Phase transitions and thermodynamic properties of yttria, Y<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O<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>: Inelastic neutron scattering shell model and first-principles calculations. Physical Review B, 2011, 84, .	1.1	35
7	Phonons, nature of bonding, and their relation to anomalous thermal expansion behavior of M2O (M) Tj ETQq1 1 0.784314 rgBT /Ove	1.1	30
8	Raman and ab initio investigation of negative thermal expansion material TaVO5: Insights into phase stability and anharmonicity. Journal of Applied Physics, 2015, 117, .	1.1	28
9	Suppression of antiferroelectric state in NaNbO3 at high pressure from in situ neutron diffraction. Applied Physics Letters, 2012, 101, .	1.5	27
10	Lattice dynamics and thermal expansion behavior in the metal cyanides<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>M</mml:mi><mml:mi>CN</mml:mi></mml:mrow></mml:	1.1	26
11	Magnetic lattice dynamics of the oxygen-free FeAs pnictides: how sensitive are phonons to magnetic ordering?. Journal of Physics Condensed Matter, 2010, 22, 315701.	0.7	24
12	Inelastic neutron scattering studies of phonon spectra, and simulations of pressure-induced amorphization in tungstates<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>A</mml:mi><mml:mi mathvariant="normal">W</mml:mi><mml:msub><mml:mi		

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19	Symmetries of modes in Ni₃V₂O₈: Polarized Raman spectroscopy and ab initio phonon calculations. Journal of Raman Spectroscopy, 2019, 50, 587-594.	1.2	17
20	Correlation of octahedral distortion with vibrational and electronic properties of LaFe1-Ti O3 nanoparticles. Journal of Alloys and Compounds, 2020, 830, 154594.	2.8	17
21	Vibrational properties and phase transitions in IIâ€“VI materials: lattice dynamics,ab initiostudies and inelastic neutron scattering measurements. Journal of Physics Condensed Matter, 2012, 24, 115401.	0.7	16
22	Dynamical and elastic properties of MgSiO₃ perovskite (bridgmanite). Geophysical Research Letters, 2016, 43, 2568-2575.	1.5	15
23	Lithium diffusion in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">L</mml:mi><mml:msub><mml:mi mathvariant="normal">i</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>X</mml:mi></mml:mrow></mml:math>		

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37	n of sodium ions in amorphous<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">N</mml:mi><mml:msub><mml:mi mathvariant="normal">a</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:msub><mml:mi	0.9	10
38	Spin-phonon coupling and high-pressure phase transitions of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>R</mml:mi><mml:mi>Mn</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>(<mml:math)	1.1	9
39	Investigating anomalous thermal expansion of copper halides by inelastic neutron scattering and ab initio phonon calculations. Physical Chemistry Chemical Physics, 2017, 19, 12107-12116.	1.3	9
40	Phonons, phase transitions and thermal expansion in LiAlO₂: an ab initio density functional study. Physical Chemistry Chemical Physics, 2018, 20, 12248-12259.	1.3	9
41	Ultra-low thermal conductivity of orthorhombic CH3NH3SnI3: A first principles investigation. Journal of Solid State Chemistry, 2020, 290, 121541.	1.4	9
42	High-temperature phonon spectra of multiferroic BiFeO3 from inelastic neutron spectroscopy. Applied Physics Letters, 2012, 100, .	1.5	8
43	Inelastic neutron scattering an ab-initio calculation of negative thermal expansion in Ag2O. Physica B: Condensed Matter, 2012, 407, 2146-2149.	1.3	8
44	Phonons and anomalous thermal expansion behavior of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">D</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">	1.1	8
45	Phase transitions in delafossite CuLaO2 at high pressures. Journal of Applied Physics, 2014, 115, .	1.1	7
46	Evidence of lowâ€temperature phase transition in BaTiO₃â€modified NaNbO₃: Raman spectroscopy study. Journal of Raman Spectroscopy, 2019, 50, 1949-1955.	1.2	7
47	Defect topology and annihilation by cooperative movement of atoms in neutron-irradiated graphite. Physical Review B, 2020, 102, .	1.1	7
48	Structural change from Pbnm to R3Ì…c phase with varying Fe/Mn content in (1-x) LaFeO3.xLaMnO3 solid solution leading to modifications in octahedral tilt and valence states. Journal of Alloys and Compounds, 2021, 883, 160761.	2.8	7
49	Evidence for anharmonic behavior of Cu diffusion in superionic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Cu</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">X</mml:mi></mml:mrow></mml:math> <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>(</mml:mo><mml:mi>X</mml:mi><mml:mo>=	0.9	7
50	New insights into the compressibility and high-pressure stability of Ni(CN)2: a combined study of neutron diffraction, Raman spectroscopy, and inelastic neutron scattering. Journal of Physics Condensed Matter, 2016, 28, 045402.	0.7	6
51	Phonons and Thermal Expansion Behavior of NiSi and NiGe. Frontiers in Chemistry, 2018, 6, 331.	1.8	6
52	High pressure behavior of complex phosphate K2Ce[PO4]2: GrÃ¼neisen parameter and anharmonicity properties. Journal of Solid State Chemistry, 2018, 258, 845-853.	1.4	5
53	Orbital- and atom-dependent linear dispersion across the Fermi level induces charge density wave instability in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>EuTe</mml:mi><mml:mn>4</mml:mn></mml:msub> Physical Review B, 2022, 105, .	1.1	5
54	High Pressure Phase Transitions in Yttria, Y₂O₃. Journal of Physics: Conference Series, 2012, 377, 012036.	0.3	4

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55	Preparation, crystal structure, vibrational and electronic properties of Cd4Si2O7F2. Journal of Alloys and Compounds, 2017, 702, 573-584.	2.8	4
56	Structural, elastic, vibrational and optical properties of energetic material octanitrocubane studied from first-principles theory. Journal of Physics Condensed Matter, 2020, 32, 425502.	0.7	4
57	Stoichiometric tuning of lattice flexibility and Na diffusion in NaAlSiO₄: quasielastic neutron scattering experiment and ab initio molecular dynamics simulations. Journal of Materials Chemistry A, 2021, 9, 16129-16136.	5.2	4
58	Comparative study of electronic structure, optical properties, lattice dynamics and thermal expansion behaviour of energetic ammonium and potassium dinitramide salts. Materials Chemistry and Physics, 2021, 267, 124645.	2.0	4
59	Presence of water at elevated temperatures, structural transition, and thermal expansion behavior in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>LaP</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:mo>:</mml:mo><mml:mi>Eu</mml:mi></mml:mrow></ Physical Review Materials, 2018, 2, .	0.9	4
60	Sodium diffusion and dynamics in Na₂Ti₃O₇: neutron scattering and ab initio simulations. Materials Advances, 2022, 3, 2104-2116.	2.6	4
61	Evidence of Spin Resonance Signal in Oxygen Free Superconducting CaFe_{0.88}Co_{0.12}AsF: An Inelastic Neutron Scattering Study. Journal of the Physical Society of Japan, 2013, 82, 104716.	0.7	3
62	Density Functional Studies Revealing Anomalous Lattice Behavior in Metal Cyanide, AgC₈N₅. Journal of Physical Chemistry C, 2018, 122, 15575-15581.	1.5	3
63	Comment on â€œInterplay between Phonons and Anisotropic Elasticity Drives Negative Thermal Expansion in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>PbTiO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn â€• Physical Review Letters, 2019, 123, 179601.	2.9	3
64	Spinâ€“phonon coupling and thermodynamic behaviour in YCrO₃ and LaCrO₃: inelastic neutron scattering and lattice dynamics. Journal of Physics Condensed Matter, 2020, 32, 505402.	0.7	3
65	Effect of hydration and ammonization on the thermal expansion behavior of ZrW2O8 : Ab initio lattice dynamical perspective. Physical Review B, 2018, 98, .	1.1	2
66	Phonons and anisotropic thermal expansion behavior of NiX (Xâ€‰=â€‰S, Se, Te). Journal of Applied Physics, 2019, 125, .	1.1	2
67	Phonons and Anomalous Lattice Behavior in KMnAg₃(CN)₆ and KNiAu₃(CN)₆: Inelastic Neutron Scattering and First-Principles Calculations. Journal of Physical Chemistry C, 2020, 124, 7216-7228.	1.5	2
68	Magnetoelastic coupling and spin contributions to entropy and thermal transport in biferroic yttrium orthochromite [*]. Journal of Physics Condensed Matter, 2021, 33, 125702.	0.7	2
69	Breaking of inversion symmetry in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>NdGa</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2021, 103, .	1.1	2
70	Phonons and oxygen diffusion in Bi2O3 and (Bi0.7Y0.3)2O3. Journal of Physics Condensed Matter, 2020, 32, 334002.	0.7	2
71	Topological phonons and electronic structure of Li₂BaSi class of semimetals. Journal of Physics Condensed Matter, 2022, 34, 125502.	0.7	2
72	Reversible optical control of Fano resonance and domain configuration at room temperature in BaTiO3. Journal of Applied Physics, 2022, 131, 053102.	1.1	2

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73	Phonons and stability of infinite-layer iron oxides SrFeO2 and CaFeO2. Solid State Communications, 2016, 241, 43-55.	0.9	1
74	Anomalous Lattice Dynamics in AgC4N3: Insights From Inelastic Neutron Scattering and Density Functional Calculations. Frontiers in Chemistry, 2018, 6, 544.	1.8	1
75	Anharmonic phonons and anomalous thermal expansion of graphite. Solid State Communications, 2021, 332, 114324.	0.9	1
76	Phase transition mechanism of hexagonal graphite to hexagonal and cubic diamond: ab initio simulation. Journal of Physics Condensed Matter, 2021, 33, 425403.	0.7	1
77	Neutron irradiation induced magnetization and persistent defects at high temperatures in graphite. Physical Review B, 2022, 105, .	1.1	1
78	Ab-initio Studies Of Lithium Oxide. , 2010, , .		0
79	Inelastic Neutron Scattering and Ab-Initio Calculation of Negative Thermal Expansion in Ag[sub 2]O. , 2011, , .		0
80	Fast ion conduction and phonon instability in lithium oxide. , 2012, , .		0
81	Inelastic neutron scattering investigations of negative thermal expansion behavior in semiconductors and framework solids. Neutron News, 2014, 25, 34-37.	0.1	0
82	Strong trilinear coupling of phonon instabilities drives the avalanche-like hybrid improper ferroelectric transition in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>SrBi</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>9</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2021, 103, .	1.1	0
83	High thermopower and birefringence in layered mercury-based halides. Materials Today Communications, 2022, 32, 102824.	0.9	0
84	Scattering lifetime and High figure of merit in CsAgO predicted by methods beyond relaxation time approximation. Journal of Physics Condensed Matter, 2022, , .	0.7	0