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	High thermopower and birefringence in layered mercury-based halides. Materials Today Communications, 2022, 32, 102824.	0.9	0
2	Topological phonons and electronic structure of Li₂BaSi class of semimetals. Journal of Physics Condensed Matter, 2022, 34, 125502.	0.7	2
3	Sodium diffusion and dynamics in Na₂Ti₃O₇: neutron scattering and ab initio simulations. Materials Advances, 2022, 3, 2104-2116.	2.6	4
4	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></mm Physical Review B, 2022, 105, .	1.1	5
5	Reversible optical control of Fano resonance and domain configuration at room temperature in BaTiO3. Journal of Applied Physics, 2022, 131, 053102.	1.1	2
6	Neutron irradiation induced magnetization and persistent defects at high temperatures in graphite. Physical Review B, 2022, 105, .	1.1	1
7	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
8	Solidlike to liquidlike 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: 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
9	: A. Physical Review Materials, 2022, 6, . 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
10	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
11	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
12	Quasi-One-Dimensional Fermi Surface Nesting and Hidden Nesting Enable Multiple Kohn Anomalies in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math> -Uranium. Physical Review Letters, 2021, 126, 096401.	2.9	12
13	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
14	Phonons and lithium diffusion in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LiAlO</mml:mi><mml:mn>2</mml:mn></mml:msub></mm Physical Review B, 2021, 103, .	1.1	11
15	Anharmonic phonons and anomalous thermal expansion of graphite. Solid State Communications, 2021, 332, 114324.	0.9	1
16	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
17	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
18	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

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19	Ultra-low thermal conductivity of orthorhombic CH3NH3SnI3: A first principles investigation. Journal of Solid State Chemistry, 2020, 290, 121541.	1.4	9
20	Defect topology and annihilation by cooperative movement of atoms in neutron-irradiated graphite. Physical Review B, 2020, 102, .	1.1	7
21	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
22	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
23	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
24	Diffusion 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 mathvariant="normal">i</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant	0.9	10
25	Phonons and oxygen diffusion in Bi2O3 and (Bi0.7Y0.3)2O3. Journal of Physics Condensed Matter, 2020, 32, 334002.	0.7	2
26	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
27	Phonons and anisotropic thermal expansion behavior of NiX (Xâ€‰=â€‰S, Se, Te). Journal of Applied Physics, 2019, 125, .	1.1	2
28	Evidence of lowâ€temperature phase transition in BaTiO₃â€modified NaNbO₃: Raman spectroscopy study. Journal of Raman Spectroscopy, 2019, 50, 1949-1955.	1.2	7
29	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	2.9	3
30	Negative thermal expansion behavior in orthorhombic Sc2(MoO4)3 and Sc2(WO4)3. Journal of Applied Physics, 2019, 126, 125114.	1.1	11
31	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	Phonons and anomalous thermal expansion behaviour in crystalline solids. Progress in Materials Science, 2018, 92, 360-445.	16.0	116
38	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
39	Phonons and Thermal Expansion Behavior of NiSi and NiGe. Frontiers in Chemistry, 2018, 6, 331.	1.8	6
40	Anomalous Lattice Dynamics in AgC4N3: Insights From Inelastic Neutron Scattering and Density Functional Calculations. Frontiers in Chemistry, 2018, 6, 544.	1.8	1
41	Phonons and anomalous thermal expansion behavior in <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
42	Detail investigations of SmFeO 3 under extreme condition. Materials Chemistry and Physics, 2018, 215, 393-403.	2.0	10
43	Density Functional Studies Revealing Anomalous Lattice Behavior in Metal Cyanide, AgC₈N₅. Journal of Physical Chemistry C, 2018, 122, 15575-15581.	1.5	3
44	Negative thermal expansion behavior in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>M</mml:mi><mml:mi>Zr</mml:mi><mml:msub><mml:mi mathvariant="normal">F</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:mrow><mml:mspace width="4pt" /><mml:mo>(</mml:mo><mml:mrow><mml:mi>M</mml:mi><mml:mo>=</mml:mo><mml:mi>Ca</mml:mi><mml:mo>,</mml:mo><mm	1.1	13
45	Presence of water at elevated temperatures, structural transition, and thermal expansion behavior in : Ab initio lattice dynamical stud. Physical Review B, 2018, 98, . <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>LaP</mml:mi><mml:msub><mml:mi>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
46	Phase Transformation, Vibrational and Electronic Properties of K₂Ce(PO₄)₂: A Combined Experimental and Theoretical Study. Inorganic Chemistry, 2017, 56, 3335-3348.	1.9	14
47	Preparation, crystal structure, vibrational and electronic properties of Cd4Si2O7F2. Journal of Alloys and Compounds, 2017, 702, 573-584.	2.8	4
48	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
49	Anomalous lattice behavior of vanadium pentaoxide (V₂O₅): X-ray diffraction, inelastic neutron scattering and ab initio lattice dynamics. Physical Chemistry Chemical Physics, 2017, 19, 17967-17984.	1.3	20
50	Superionic conduction in Î²-eucryptite: inelastic neutron scattering and computational studies. Physical Chemistry Chemical Physics, 2017, 19, 15512-15520.	1.3	14
51	Role of phonons in negative thermal expansion and high pressure phase transitions in Î²-eucryptite: An ab-initio lattice dynamics and inelastic neutron scattering study. Journal of Applied Physics, 2017, 121, .	1.1	14
52	Anomalous thermal expansion, negative linear compressibility, and high-pressure phase transition in ZnAu2(CN)4 : Neutron inelastic scattering and lattice dynamics studies. Physical Review B, 2017, 96, .	1.1	13
53	Effect of Preparation Conditions on Magnetic and Dielectric Properties of Y₂MMnO₆ (M = Co, Ni). Journal of the American Ceramic Society, 2016, 99, 499-506.	1.9	21
54	Phonons and stability of infinite-layer iron oxides SrFeO2 and CaFeO2. Solid State Communications, 2016, 241, 43-55.	0.9	1

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55	Dynamical and elastic properties of MgSiO₃ perovskite (bridgmanite). Geophysical Research Letters, 2016, 43, 2568-2575.	1.5	15
56	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
57	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	0.7843
58	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
59	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
60	Spin-phonon coupling and high-temperature phase transition in multiferroic material YMnO₃. Journal of Materials Chemistry C, 2015, 3, 11717-11728.	2.7	12
61	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
62	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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73	High Pressure Phase Transitions in Yttria, Y₂O₃. Journal of Physics: Conference Series, 2012, 377, 012036.	0.3	4
74	Suppression of antiferroelectric state in NaNbO3 at high pressure from in situ neutron diffraction. Applied Physics Letters, 2012, 101, .	1.5	27
75	High-temperature phonon spectra of multiferroic BiFeO3 from inelastic neutron spectroscopy. Applied Physics Letters, 2012, 100, .	1.5	8
76	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
77	Phonon instability and mechanism of superionic conduction in Li<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. Physical Review B, 2012, 85, .	1.1	19
78	Inelastic neutron scattering an ab-initio calculation of negative thermal expansion in Ag2O. Physica B: Condensed Matter, 2012, 407, 2146-2149.	1.3	8
79	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
80	Inelastic Neutron Scattering and Ab-Initio Calculation of Negative Thermal Expansion in Ag[sub 2]O. , 2011, , .		0
81	Ab-initio Studies Of Lithium Oxide. , 2010, , .		0
82	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
83	Ab initiolattice 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
84	Inelastic neutron scattering and lattice dynamics of minerals. European Journal of Mineralogy, 2002, 14, 291-329.	0.4	76