Manish Kumar Niranjan

List of Publications by Year
in descending order

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63	2,180	331538	223716
papers	citations	21 h-index	46 g-index

64	64	64	2888
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Improved electronic structure prediction of chalcopyrite semiconductors from a semilocal density functional based on Pauli kinetic energy enhancement factor. Journal of Physics Condensed Matter, 2022, 34, 075501.	0.7	3
2	Chalcogen dependent metal vacancies and disorder in Ba2Ln1â^'Mn2â^'S5 and Ba2â^'Ln1â^'Mn2â^'Se5 (LnÂ=ÂPr,) Tj ETQq0 0 0 rgBT /Ov	2.8	2
3	Germanium Antimony Bonding in Ba₄Ge₂Sb₂Te₁₀ with Low Thermal Conductivity. Inorganic Chemistry, 2022, 61, 968-981.	1.9	10
4	Synthesis, crystal structure, optical bandgap, and electronic structure of Cs2FeP2S6. Solid State Sciences, 2022, , 106891.	1.5	1
5	Influence of phonon-assisted tunneling on photovoltaic properties of BaSi2 and BaGe2â€^pâ€"n homojunction solar cell devices. Journal of Applied Physics, 2022, 131, .	1.1	1
6	Interface magnetoelectric effect and its sensitivity on interface structures in Fe/AgNbO3 and SrRuO3/AgNbO3 heterostructures: A first-principles investigation. Journal of Magnetism and Magnetic Materials, 2021, 517, 167372.	1.0	2
7	Syntheses of five new layered quaternary chalcogenides SrScCuSe₃, SrScCuTe₃, BaScCuSe₃, BaScCuTe₃, and BaScAgTe₃: crystal structures, thermoelectric properties, and electronic structures. Inorganic Chemistry Frontiers, 2021, 8, 4086-4101.	3.0	37
8	Ba₂Ln_{1â^'x}Mn₂Te₅ (Ln = Pr, Gd, and Yb; x = Ln) Tj ETQq0 0 0 rgBT /Overlock Transactions, 2021, 50, 6688-6701.	1.6	8
9	Significance of Coulomb interaction in interlayer coupling, polarized Raman intensities, and infrared activities in the layered van der Waals semiconductor GaSe. Physical Review B, 2021, 103, .	1.1	6
10	Theoretical investigation of lattice dynamics, infrared reflectivity, polarized Raman spectra and nature of interlayer coupling in two-dimensional layered gallium sulfide. Journal of Physics Condensed Matter, 2021, 33, 405001.	0.7	1
11	Reactive molten-flux assisted syntheses of single crystals of Cs19Ln19Mn10Te48 (Ln = Pr and Gd) crystallizing in a new structure type. CrystEngComm, 2021, 23, 8418-8429.	1.3	2
12	Surface electronic structure, relaxations and thermodynamic energies of (100), (110) and (111) surfaces of Mg2Si: A first-principles theoretical study. Surface Science, 2020, 691, 121506.	0.8	4
13	Synthesis, crystal structure, optical absorption study, and electronic structure of Cs3FeCl5. Solid State Sciences, 2020, 100, 106064.	1.5	6
14	Schottky barrier height and modulation due to interface structure and defects in Pt|MgO|Pt heterojunctions with implications for resistive switching. Journal of Applied Physics, 2020, 127, 205306.	1.1	1
15	Surface electronic structure, thermodynamic stability of Na1/2Bi1/2TiO3 (001) surfaces and their relevance to A-site cation ordering in bulk phases: A first-principles study. Solid State Sciences, 2020, 102, 106161.	1.5	1
16	First principle study of bias voltage dependent Schottky barrier height of Pt/MgO interface. AIP Conference Proceedings, 2020, , .	0.3	1
17	Theoretical investigation of electronic bandgaps of semiconducting single-walled carbon nanotubes using semi-empirical self-consistent tight binding and ab-inito density functional methods. Journal of Physics Communications, 2020, 4, 015004.	0.5	16
18	Large modulation of interface magnetization and interface magnetoelectric effect in SrRuO3|KNbO3 oxide heterostructures: Prediction from first-principles study. Journal of Magnetism and Magnetic Materials, 2019, 469, 138-145.	1.0	5

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19	Theoretical investigation of surface electronic structure and thermodynamic energies of (1x1) polar and nonpolar K1/2Bi1/2TiO3 (001) surfaces. Journal of Physics and Chemistry of Solids, 2019, 135, 109116.	1.9	2
20	Asymmetric-dimer reconstruction and semiconducting properties of Mg2Si(100) surfaces: Prediction from meta-GGA and hybrid functional study. Solid State Sciences, 2019, 98, 106030.	1.5	1
21	Theoretical investigation of lattice dynamics, dielectric properties, infrared reflectivity and Raman intensity spectra of Nowotny chimney-ladder semiconducting silicide Ru2Si3. Materials Chemistry and Physics, 2019, 222, 165-172.	2.0	4
22	Optimum discharge energy density at room temperature in relaxor K_{1/2}Bi_{1/2}TiO₃for green energy harvesting. Journal Physics D: Applied Physics, 2018, 51, 115501.	1.3	17
23	Interface Local Magnetic Moment and Its Near Periodic Modulation in Oxide SrRuO₃|LaAlO₃ Heterojunctions: An <italic>Ab Initio</italic> Investigation. IEEE Transactions on Magnetics, 2018, 54, 1-7.	1.2	1
24	Phonon modes, dielectric properties, infrared reflectivity, and Raman intensity spectra of semiconducting silicide BaSi2: First principles study. Journal of Physics and Chemistry of Solids, 2018, 121, 219-227.	1.9	5
25	Randomly arranged cation-ordered nanoregions in lead-free relaxor ferroelectric K1/2Bi1/2TiO3: Prediction from first-principles study. Journal of Applied Physics, 2018, 123, .	1.1	8
26	Electronic structure, vibrational and thermoelectric properties of AgTaO3: A first-principles study. Journal of Alloys and Compounds, 2017, 696, 1168-1173.	2.8	11
27	The electrical properties and relaxation behavior of AgNb1/2Ta1/2O3 ceramic. Physica B: Condensed Matter, 2017, 506, 42-47.	1.3	7
28	Phase stability and elastic properties ofÎ²Tiâ€“Nbâ€“X(X= Zr, Sn) alloys: anab initiodensity functional study. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 085013.	0.8	10
29	Precise control of Schottky barrier height in SrTiO₃/SrRuO₃heterojunctions using ultrathin interface polar layers. Journal Physics D: Applied Physics, 2016, 49, 255302.	1.3	5
30	Infrared reflectivity and Raman intensity spectrum of relaxor ferroelectric Na1/2Bi1/2TiO3at room temperature: a first-principles theoretical study. Materials Research Express, 2016, 3, 125501.	0.8	2
31	Aliovalent cation ordering, coexisting ferroelectric structures, and electric field induced phase transformation in lead-free ferroelectric Na0.5Bi0.5TiO3. Journal of Applied Physics, 2016, 119, .	1.1	10
32	Investigation of Raman Modes and Bornâ€Effective Charges in AgNb_{1/2}Ta_{1/2}O₃: A Densityâ€Functional and Raman Scattering Study. Journal of the American Ceramic Society, 2016, 99, 332-339.	1.9	10
33	Theoretical investigation of surface states and energetics of PtSi surfaces. Surface Science, 2016, 649, 27-33.	0.8	4
34	Interface electronic structure and Schottky-barrier height in Si/NiSi(010) and Si/PtSi(010) heterostructures: A first-principles theoretical study. Superlattices and Microstructures, 2016, 100, 808-817.	1.4	2
35	The structural and electronic properties of cubic AgMO3 (M=Nb, Ta) by first principles calculations. AIP Conference Proceedings, 2016, , .	0.3	2
36	Microstructural studies of AgNbO3 ceramic by using complex impedance spectroscopy. AIP Conference Proceedings, 2015, , .	0.3	6

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37	Investigation of structural, vibrational and ferroic properties of AgNbO₃at room temperature using neutron diffraction, Raman scattering and density-functional theory. Journal Physics D: Applied Physics, 2015, 48, 215303.	1.3	25
38	First principles theoretical investigations of low Young's modulus beta Tiâ€“Nb and Tiâ€“Nbâ€“Zr alloys compositions for biomedical applications. Materials Science and Engineering C, 2015, 50, 52-58.	3.8	100
39	Observation of coexistence of ferroelectric and antiferroelectric phases in Sc substituted BiFeO3. Journal of Alloys and Compounds, 2015, 642, 192-199.	2.8	18
40	Anisotropy in elastic properties of TiSi₂(C49,C40 andC54), TiSi and Ti₅Si₃: anab-initiodensity functional study. Materials Research Express, 2015, 2, 096302.	0.8	10
41	Ab-initio determination of thermodynamic properties of CoSi2. Computational Materials Science, 2014, 95, 517-521.	1.4	5
42	Effect of surface structure on workfunction and Schottky-barrier height in SrRuO3/SrTiO3 (001) heterojunctions. Journal of Applied Physics, 2014, 115, 173705.	1.1	21
43	Enhancement of magnetic and electrical properties in Sc substituted BiFeO3 multiferroic. Physica B: Condensed Matter, 2014, 448, 267-272.	1.3	40
44	Gruneisen parameter and thermal expansion coefficients of NiSi₂from first-principles. Journal Physics D: Applied Physics, 2014, 47, 285101.	1.3	8
45	Theoretical and experimental investigation of Raman modes, ferroelectric and dielectric properties of relaxor Na0.5Bi0.5TiO3. Journal of Applied Physics, 2013, 113, .	1.1	183
46	Relation between the work function and Young's modulus of RhSi and estimate of Schottky-barrier height at RhSi/Si interface: An ab-initio study. Journal of Applied Physics, 2012, 112, .	1.1	11
47	First principles study of lead free piezoelectric AgNbO3 and (Ag1â^'xKx)NbO3 solid solutions. Solid State Communications, 2012, 152, 1707-1710.	0.9	40
48	First principles study of structural, electronic and elastic properties of cubic and orthorhombic RhSi. Intermetallics, 2012, 26, 150-156.	1.8	26
49	Synthesis of oxidation resistant copper nanoparticles in aqueous phase and efficient phase transfer of particles using alkanethiol. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2012, 407, 58-63.	2.3	26
50	Metallic and Insulating Oxide Interfaces Controlled by Electronic Correlations. Science, 2011, 331, 886-889.	6.0	212
51	Electric field effect on magnetization at the Fe/MgO(001) interface. Applied Physics Letters, 2010, 96, .	1.5	270
52	Prediction of a Switchable Two-Dimensional Electron Gas at Ferroelectric Oxide Interfaces. Physical Review Letters, 2009, 103, 016804.	2.9	115
53	First-principles studies of a two-dimensional electron gas at the interface in ferroelectric oxide heterostructures. Physical Review B, 2009, 80, .	1.1	34
54	Prediction of a spin-polarized two-dimensional electron gas at theLaAlO3/EuO(001)interface. Physical Review B, 2009, 79, .	1.1	44

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55	Magnetoelectric effect at the SrRuO3/BaTiO3 (001) interface: An ab initio study. Applied Physics Letters, 2009, 95, .	1.5	119
56	Magnetic Tunnel Junctions with Ferroelectric Barriers: Prediction of Four Resistance States from First Principles. Nano Letters, 2009, 9, 427-432.	4.5	305
57	Magnetoelectric effect at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Fe</mml:mtext></mml:mrow><mml:mn>3</mml:mn> interface: A first-principles study. Physical Review B, 2008, 78, .	1.1	155
58	Ab initiostudy of atomic structure and Schottky barrier height at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>GaAs</mml:mtext><mml:mo>/</mml:mo><mml:msub><mml:mrow><mml:mtext>Ni</mml:mtext> Physical Review B, 2008, 77, .	1.1	11
59	Electronic structure, elastic properties, surface energies, and work functions ofNiGeandPtGewithin the framework of density-functional theory for various surface terminations. Physical Review B, 2007, 75, .	1.1	23
60	Effect of spin-orbit coupling on small platinum nanoclusters. Physical Review A, 2006, 73, .	1.0	83
61	Theoretical investigation of Pt monosilicide and several germanides: electronic structure, surface energetics, and work functions. Materials Research Society Symposia Proceedings, 2006, 980, 43.	0.1	0
62	Theoretical investigation ofPtSisurface energies and work functions. Physical Review B, 2006, 73, .	1.1	41
63	Density functional determination of the magnetic state of$\hat{I}^2$-MnAs. Physical Review B, 2004, 70, .	1.1	41