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	Magnetic Tunnel Junctions with Ferroelectric Barriers: Prediction of Four Resistance States from First Principles. Nano Letters, 2009, 9, 427-432.	4.5	305
2	Electric field effect on magnetization at the Fe/MgO(001) interface. Applied Physics Letters, 2010, 96, .	1.5	270
3	Metallic and Insulating Oxide Interfaces Controlled by Electronic Correlations. Science, 2011, 331, 886-889.	6.0	212
4	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
5	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></mml:msub> interface: A first-principles study. Physical Review B, 2008, 78, .	1.1	155
6	Magnetoelectric effect at the SrRuO3/BaTiO3 (001) interface: An ab initio study. Applied Physics Letters, 2009, 95, .	1.5	119
7	Prediction of a Switchable Two-Dimensional Electron Gas at Ferroelectric Oxide Interfaces. Physical Review Letters, 2009, 103, 016804.	2.9	115
8	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
9	Effect of spin-orbit coupling on small platinum nanoclusters. Physical Review A, 2006, 73, .	1.0	83
10	Prediction of a spin-polarized two-dimensional electron gas at theLaAlO3/EuO(001)interface. Physical Review B, 2009, 79, .	1.1	44
11	Density functional determination of the magnetic state ofÎ²-MnAs. Physical Review B, 2004, 70, .	1.1	41
12	Theoretical investigation ofPtSisurface energies and work functions. Physical Review B, 2006, 73, .	1.1	41
13	First principles study of lead free piezoelectric AgNbO3 and (Ag1â^'xKx)NbO3 solid solutions. Solid State Communications, 2012, 152, 1707-1710.	0.9	40
14	Enhancement of magnetic and electrical properties in Sc substituted BiFeO3 multiferroic. Physica B: Condensed Matter, 2014, 448, 267-272.	1.3	40
15	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
16	First-principles studies of a two-dimensional electron gas at the interface in ferroelectric oxide heterostructures. Physical Review B, 2009, 80, .	1.1	34
17	First principles study of structural, electronic and elastic properties of cubic and orthorhombic RhSi. Intermetallics, 2012, 26, 150-156.	1.8	26
18	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

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19	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
20	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
21	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
22	Observation of coexistence of ferroelectric and antiferroelectric phases in Sc substituted BiFeO3. Journal of Alloys and Compounds, 2015, 642, 192-199.	2.8	18
23	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
24	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
25	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
26	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
27	Electronic structure, vibrational and thermoelectric properties of AgTaO3: A first-principles study. Journal of Alloys and Compounds, 2017, 696, 1168-1173.	2.8	11
28	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
29	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
30	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
31	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
32	Germanium Antimony Bonding in Ba₄Ge₂Sb₂Te₁₀ with Low Thermal Conductivity. Inorganic Chemistry, 2022, 61, 968-981.	1.9	10
33	Gruneisen parameter and thermal expansion coefficients of NiSi₂from first-principles. Journal Physics D: Applied Physics, 2014, 47, 285101.	1.3	8
34	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
35	Ba₂Ln_{1â^'x}Mn₂Te₅ (Ln = Pr, Gd, and Yb; x = Ln) Tj ETQq1 1 0.784314 rgB Transactions, 2021, 50, 6688-6701.	1.6	8
36	The electrical properties and relaxation behavior of AgNb1/2Ta1/2O3 ceramic. Physica B: Condensed Matter, 2017, 506, 42-47.	1.3	7

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37	Microstructural studies of AgNbO3 ceramic by using complex impedance spectroscopy. AIP Conference Proceedings, 2015, , .	0.3	6
38	Synthesis, crystal structure, optical absorption study, and electronic structure of Cs3FeCl5. Solid State Sciences, 2020, 100, 106064.	1.5	6
39	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
40	Ab-initio determination of thermodynamic properties of CoSi2. Computational Materials Science, 2014, 95, 517-521.	1.4	5
41	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
42	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
43	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
44	Theoretical investigation of surface states and energetics of PtSi surfaces. Surface Science, 2016, 649, 27-33.	0.8	4
45	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
46	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
47	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
48	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
49	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
50	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
51	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
52	The structural and electronic properties of cubic AgMO3 (M=Nb, Ta) by first principles calculations. AIP Conference Proceedings, 2016, , .	0.3	2
53	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
54	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

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55	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
56	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
57	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
58	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
59	First principle study of bias voltage dependent Schottky barrier height of Pt/MgO interface. AIP Conference Proceedings, 2020, , .	0.3	1
60	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
61	Synthesis, crystal structure, optical bandgap, and electronic structure of Cs2FeP2S6. Solid State Sciences, 2022, , 106891.	1.5	1
62	Influence of phonon-assisted tunneling on photovoltaic properties of BaSi2 and BaGe2â€ˆpâ€“n homojunction solar cell devices. Journal of Applied Physics, 2022, 131, .	1.1	1
63	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