Surya Chattopadhyaya

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4098332/publications.pdf

Version: 2024-02-01

41 papers	148 citations	1307594 7 h-index	1372567 10 g-index
41 all docs	41 docs citations	41 times ranked	81 citing authors

#	Article	IF	Citations
1	Tuning of optoelectronic and transport properties of zinc-blend magnesium chalcogenides through doping of Hg atom(s): The mBJ-GGA+U based first-principle calculations. Computational Condensed Matter, 2022, 30, e00650.	2.1	3
2	Investigation of structural, mechanical and optoelectronic properties of cubic Cd1â^'xâ^'yZnxHgySe quaternary alloys through first-principle calculations. Bulletin of Materials Science, 2022, 45, 1.	1.7	0
3	First-principles calculations to investigate transformation of optically inactive zinc-blend beryllium chalcogenides to optically active semiconductor alloys through doping of Hg atom(s). Physica B: Condensed Matter, 2022, , 413881.	2.7	1
4	Density Functional Calculations of Elastic and Thermal Properties of Zinc-Blende Mercuryâ€“Cadmium-Chalcogenide Ternary Alloys. Metals and Materials International, 2021, 27, 3823-3838.	3.4	4
5	Beryllium (Be) composition dependent structural and optoelectronic characteristics of wurtzite Be Mg1-S ternary alloys: First principle calculations with FP-LAPW scheme. Materials Chemistry and Physics, 2021, 258, 123946.	4.0	0
6	Cationic and anionic composition-dependent mechanical and thermal properties of zinc-blende specimens under $${hbox {Mg}}_{x} {hbox {Zn}}_{1hbox {-}x} {hbox {S}}_{y} {hbox {Se}}_{1hbox {-}y}$$ quaternary system: calculations with density functional FP-LAPW scheme. European Physical Journal B, 2021, 94, 1.	1.5	0
7	Composition dependence in mechanical properties of zinc-blende compounds associated with the CdxZn1â€“xSyTe1â€“y system: a density functional study. Bulletin of Materials Science, 2021, 44, 1.	1.7	1
8	First-Principles Investigation of Structural, Elastic, Electronic, and Optical Properties of Cd1â^'xâ^'yZnxHgyS Quaternary Alloys. Journal of Electronic Materials, 2021, 50, 4705-4726.	2.2	0
9	Calculations of selenium and cadmium concentration dependent elastic and thermal properties of zinc-blende specimens under Cd Zn1-Se Te1- quaternary system with density functional theory. Materials Today Communications, 2021, 27, 102136.	1.9	1
10	Theoretical investigation of magnesium and selenium concentration dependent elastic properties of zinc blende specimens under the Mg Zn1-SeyTe1- quaternary system with density functional FP-LAPW approach. Mechanics of Materials, 2021, 158, 103840.	3.2	0
11	First principle calculations of structural, elastic, electronic and optical properties of cubic Cd1--Zn Hg Te triangular quaternary alloys and their compounds. Physica B: Condensed Matter, 2021, 614, 412999.	2.7	2
12	Pressure induced structural, electronic and optical properties of wurtzite beryllium monoxide (w-BeO) from first-principle calculations. Solid State Communications, 2021, 342, 114571.	1.9	0
13	First principle investigations of structural and optoelectronic features of cubic Cd Zn1â^'S Te1- quaternary semiconductor alloys. Optik, 2020, 201, 163510.	2.9	1
14	Calculations of the structural and optoelectronic properties of cubic CdxZn1â^'xSeyTe1â^'y semiconductor quaternary alloys using the DFT-based FP-LAPW approach. Journal of Computational Electronics, 2020, 19, 1-25.	2.5	8
15	Structural, mechanical and optoelectronic features of cubic Mg Cd1â^'S, Mg Cd1â^'Se and Mg Cd1â^'Te semiconductor ternary alloys: Theoretical investigations using density functional FP-LAPW approach. Computational Condensed Matter, 2020, 22, e00448.	2.1	5
16	Density Functional Investigations of Structural, Mechanical and Optoelectronic Properties of BeSxSe1â^'x, BeSxTe1â^'x and BeSexTe1â^'x Ternary Alloys. Journal of Electronic Materials, 2020, 49, 1372-1386.	2.2	2
17	Cationic and anionic concentration dependent elastic properties of zinc blende specimens within Cd Zn1-S Se1- quaternary system: Calculations with density functional theory. Solid State Communications, 2020, 322, 114050.	1.9	3
18	First-principle calculations of structural and optoelectronic properties of cubic CdxZn1â^'xSySe1â^'y quaternary alloys with modified Beckeâ€“Johnson (mBJ) functional. Indian Journal of Physics, 2020, , 1.	1.8	0

#	Article	IF	Citations
19	Density functional study on structural and optoelectronic properties of cubic $$hbox {Mg}_{x}hbox {Zn}_{1-x}hbox {S}_{y}hbox {Se}_{1-y}$$ semiconductor quaternary alloys. Pramana - Journal of Physics, 2020, 94, 1.	1.8	2
20	Density functional study of elastic and thermal properties of cubic mercury-zinc-chalcogenide ternary alloys. Bulletin of Materials Science, 2020, 43, 1.	1.7	1
21	Structural, mechanical and optoelectronic properties of cubic $$hbox {Be}_{x}hbox {Mg}_{1-x}hbox {S}, hbox {Be}_{x}hbox {Mg}_{1-x}hbox {Se}$$ and $$hbox {Be}_{x}hbox {Mg}_{1-x}hbox {Te}$$ semiconductor ternary alloys: a density functional study. Bulletin of Materials Science, 2020, 43, 1.	1.7	0
22	First principles investigations of structural and optoelectronic properties of cubic MgxZn1â^'xSeyTe1â^'y quaternary semiconductor alloys using FP-LAPW approach. Applied Physics A: Materials Science and Processing, 2019, 125, 1.	2.3	1
23	Structural and optoelectronic properties of cubic Mg Zn1â^'S Te1- semiconductor quaternary alloys-a first principles investigation. Physica B: Condensed Matter, 2019, 574, 411669.	2.7	2
24	Optoelectronic properties of CaxBa1â^'xX (X=S, Se and Te) alloys: A first principles investigation employing modified Beckeâ€"Johnson (mBJ) functional. International Journal of Modern Physics B, 2019, 33, 1950042.	2.0	3
25	Density functional study of structural, elastic, electronic and optical properties of Be Cd1â^'S, Be Cd1â^'Se and Be Cd1â^'Te alloys using FP-LAPW approach. Physica B: Condensed Matter, 2019, 563, 1-22.	2.7	4
26	First principle based calculations of the optoelectronic features of HgS Se1â^', HgS Te1â^' and HgSe Te1â^' alloys with GGA+U functional. Journal of Physics and Chemistry of Solids, 2019, 131, 86-103.	4.0	11
27	Influence of doping of mercury atom(s) on optoelectronic properties of binary cadmium chalcogenides - A density functional theory based investigation with different exchange-correlation functionals and including spin-orbit coupling. Current Applied Physics, 2018, 18, 698-716.	2.4	12
28	Effects of doping of mercury atom(s) on optoelectronic properties of binary zinc chalcogenides - A first principle based theoretical investigation. Journal of Alloys and Compounds, 2018, 748, 446-463.	5.5	14
29	Tuning of electronic band gaps and optoelectronic properties of binary strontium chalcogenides by means of doping of magnesium atom(s)- a first principles based theoretical initiative with mBJ, B3LYP and WC-GGA functionals. Physica B: Condensed Matter, 2018, 530, 53-68.	2.7	3
30	Modification of band gaps and optoelectronic properties of binary calcium chalcogenides by means of doping of magnesium atom(s) in rock-salt phase- a first principle based theoretical initiative. Journal of Solid State Chemistry, 2018, 258, 358-375.	2.9	12
31	DFT based FP-LAPW investigation of structural, electronic and optical properties of Sr x Pb 1â^'x S, Sr x Pb 1â^'x Se and Sr x Pb 1â^'x Te ternary alloys. Journal of Alloys and Compounds, 2017, 698, 868-882.	5.5	3
32	Effects of barium (Ba) doping on structural, electronic and optical properties of binary strontium chalcogenide semiconductor compounds - A theoretical investigation using DFT based FP-LAPW approach. Materials Chemistry and Physics, 2017, 199, 295-312.	4.0	17
33	Theoretical study of structural, electronic and optical properties of Ba Pb1â^'S, Ba Pb1â^'Se and Ba Pb1â^'Te ternary alloys using FP-LAPW approach. Journal of Alloys and Compounds, 2017, 694, 1348-1364.	5.5	12
34	FP-LAPW methodology based theoretical investigation of structural, electronic and optical properties of MgxPb1â^'xS, MgxPb1â^'xSe and MgxPb1â^'xTe ternary alloys. Journal of Physics and Chemistry of Solids, 2017, 100, 57-70.	4.0	5
35	Effects of spinâ€"orbit coupling on the electronic states and spectroscopic properties of tellurium monoxide molecule â€" A theoretical study. Computational and Theoretical Chemistry, 2016, 1084, 75-87.	2.5	0
36	Electronic states and spectroscopic properties of MgH in absence and presence of spinâ€"orbit coupling â^' a configuration interaction study. Molecular Physics, 2016, 114, 3026-3039.	1.7	2

#	Article	IF	Citations
37	Effects of spinâ€“orbit coupling on the electronic states and spectroscopic properties of diatomic SeS. Journal of Physics B: Atomic, Molecular and Optical Physics, 2016, 49, 065101.	1.5	2
38	Theoretical investigation of electronic states and spectroscopic properties of tellurium selenide molecule employing relativistic effective core potentials. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 124, 618-628.	3.9	4
39	Theoretical studies of the electronic spectrum of tellurium monosulfide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 112, 283-289.	3.9	3
40	Configuration interaction study of the electronic states and spectroscopic properties of selenium monoxide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 89, 160-167.	3.9	4
41	First-principles investigations of composition-dependent mechanical properties of zinc-blende constituents of MgxZn1â^'xSyTe1â^'y rectangular quaternary system. Indian Journal of Physics, 0, , 1.	1.8	0