

Sikander Azam

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/441770/publications.pdf>

Version: 2024-02-01

121
papers

1,204
citations

471509

17
h-index

610901

24
g-index

124
all docs

124
docs citations

124
times ranked

828
citing authors

#	ARTICLE	IF	CITATIONS
1	Investigation of structural, electronic and optical properties of potassium and lithium based ternary Selenoindate: Using first principles approach. <i>Journal of Solid State Chemistry</i> , 2021, 293, 121778.	2.9	42
2	First-principles calculations of a half-metallic ferromagnet zinc blende Zn $1\hat{x}V \times Te$. <i>Journal of Magnetism and Magnetic Materials</i> , 2015, 378, 41-49.	2.3	40
3	Revealing the optoelectronic and thermoelectric properties of the Zintl quaternary arsenides $ACdGeAs_2$ ($A = K, Rb$). <i>Materials Research Bulletin</i> , 2015, 70, 847-855.	5.2	39
4	Tailoring the electrical properties of $MoTe_2$ field effect transistor via chemical doping. <i>Superlattices and Microstructures</i> , 2019, 135, 106247.	3.1	35
5	DFT study of the electronic and optical properties of ternary chalcogenides $AlX_2 \times Te_4$. <i>Materials Research Express</i> , 2019, 6, 116314.	1.6	33
6	Elastic and optoelectronic properties of $CaTa_2O_6$ compounds: Cubic and orthorhombic phases. <i>Journal of Alloys and Compounds</i> , 2019, 785, 232-239.	5.5	31
7	Optoelectronic structure and related transport properties of $BiCuSeO$ -based oxychalcogenides: First principle calculations. <i>Solid State Sciences</i> , 2016, 58, 86-93.	3.2	26
8	Half-metallic ferromagnetism in $Be_1\hat{x}V \times Te$ alloys: an Ab-initio study. <i>Indian Journal of Physics</i> , 2015, 89, 1251-1263.	1.8	24
9	Electronic band structure and specific features of Sm_2NiMnO_6 compound: DFT calculation. <i>Journal of Magnetism and Magnetic Materials</i> , 2013, 342, 80-86.	2.3	23
10	Electronic structure and optical properties of CdO from bulk to nanosheet: DFT approach. <i>Optical Materials</i> , 2015, 47, 372-378.	3.6	23
11	Optoelectronic and Thermoelectric Properties of Bi_2OX_2 ($X = As, Se, Te$) for Solar Cells and Thermoelectric Devices. <i>Journal of Electronic Materials</i> , 2018, 47, 2513-2518.	2.2	21
12	Effect of S and Se replacement on electronic and thermoelectric features of $BaCu_2GeQ_4$ ($Q = S, Se$) chalcogenide crystals. <i>Journal of Alloys and Compounds</i> , 2019, 790, 666-674.	5.5	21
13	Structure stability, half metallic ferromagnetism, magneto-electronic and thermoelectric properties of new zintl XC_2Bi_2 ($X = Ca, Sr$) compounds for spintronic and renewable energy applications. <i>Physica B: Condensed Matter</i> , 2021, 607, 412866.	2.7	21
14	Enhanced thermoelectric properties of $ASbO_3$ due to decreased band gap through modified becke johnson potential scheme. <i>Journal of Physics and Chemistry of Solids</i> , 2018, 119, 85-93.	4.0	19
15	Systematic studies of the structural and optoelectronic characteristics of $CaZn_2 \times X_2$ ($X = N, P, As, Sb, Bi$). <i>Materials Research Express</i> , 2018, 5, 016304.	1.6	19
16	Modified Becke-Johnson (mBJ) exchange potential investigations of the optoelectronic structure of the quaternary diamond-like semiconductors Li_2CdGeS_4 and Li_2CdSnS_4 . <i>Materials Science in Semiconductor Processing</i> , 2015, 39, 606-613.	4.0	18
17	Electronic, optical and thermoelectric properties of new metal-rich homological selenides with palladium-indium: Density functional theory and Boltzmann transport model. <i>Journal of Physics and Chemistry of Solids</i> , 2020, 138, 109229.	4.0	18
18	Effect of Nb, Ta and V replacements on electronic, optical and elastic properties of $NbCu_3Se_4$: A GGA+U study. <i>Journal of Solid State Chemistry</i> , 2021, 301, 122338.	2.9	18

#	ARTICLE	IF	CITATIONS
19	Effects of compressed strain on thermoelectric properties of Cu ₃ SbSe ₄ . Journal of Alloys and Compounds, 2018, 750, 804-810.	5.5	17
20	Electronic and Thermoelectric Properties of Ternary Chalcogenide Semiconductors: First Principles Study. Journal of Electronic Materials, 2018, 47, 1131-1139.	2.2	17
21	Effect of Coulomb interactions on optoelectronic and magnetic properties of novel A ₂ V ₂ O ₇ (A= Fe) Tj ETQq1 1 0.784314 rgBT /Over	5.5	17
22	First-principles study of opto-electronic and thermoelectric properties of SrCdSnX ₄ (X=S, Se, Te) alkali metal chalcogenides. Computational Condensed Matter, 2022, 30, e00625.	2.1	17
23	A Systematic First-Principles Investigation of Structural, Electronic, Magnetic, and Thermoelectric Properties of Thorium Monopnictides ThPn (Pn=As, N, P, As): A Comparative Analysis of Theoretical Predictions of LDA, PBEsol, PBE-GGA, WC-GGA, and LDA+U Methods. International Journal of Thermophysics, 2019, 40, 1.	2.1	16
24	Exploring the electronic structure and optical properties of new inorganic luminescent materials Ba(Si,Al) ₅ (O,N) ₈ compounds for light-emitting diodes devices. Current Applied Physics, 2015, 15, 1160-1167.	2.4	15
25	A first principles study of electronic and optical properties of the polar quaternary chalcogenides \hat{I}^2 -A ₂ Hg ₃ Ge ₂ S ₈ (A=K and Rb). Materials Science in Semiconductor Processing, 2015, 34, 250-259.	4.0	15
26	Electronic structure and optical properties of TaNO: An ab initio study. Journal of Molecular Graphics and Modelling, 2019, 92, 296-302.	2.4	15
27	First-Principles Description of the Different Phases in the Li ₂ NH Compound: Electronic Structure and Optical Properties. Journal of the Korean Physical Society, 2019, 74, 1140-1145.	0.7	15
28	First-principles investigations of metal chalcogenides Tl ₂ Hg ₃ X ₄ (X=S, Se, Te) for advanced optoelectronic and thermoelectric applications. Journal of Solid State Chemistry, 2022, 312, 123199.	2.9	15
29	First-principles study of the electronic structure, charge density, Fermi surface and optical properties of zintl phases compounds Sr ₂ ZnA ₂ (A=P, As and Sb). Journal of Magnetism and Magnetic Materials, 2013, 345, 294-303.	2.3	14
30	Doping induced effect on optical and band structure properties of Sr ₂ Si ₅ N ₈ based phosphors: DFT approach. Journal of Alloys and Compounds, 2019, 771, 1072-1079.	5.5	14
31	First-principles calculations of structural, electronic, magnetic, thermoelectric, and thermodynamic properties of BaMn ₂ P ₂ in the Anti and ferromagnetic phase. Journal of Solid State Chemistry, 2021, 302, 122388.	2.9	14
32	Linear and nonlinear optical properties of \hat{I}^{\pm} -K ₂ Hg ₃ Ge ₂ S ₈ and \hat{I}^{\pm} -K ₂ Hg ₃ Sn ₂ S ₈ compounds. Optical Materials, 2014, 37, 97-103.	3.6	13
33	Exploring the electronic structure and optical properties of the quaternary selenide compound, Ba ₄ Ga ₄ SnSe ₁₂ : For photovoltaic applications. Journal of Solid State Chemistry, 2015, 229, 260-265.	2.9	13
34	Detailed DFT studies of the electronic structure and optical properties of KBaMSe ₃ (M = As, Sb). Journal of Alloys and Compounds, 2015, 644, 91-96.	5.5	13
35	Coulomb interaction and spin-orbit coupling calculations of thermoelectric properties of the quaternary chalcogenides Tl ₂ PbXY ₄ (X = Zr, Hf and Y = S, Se). Semiconductor Science and Technology, 2015, 30, 105018.	2.0	12
36	DFT and modified Becke Johnson (mBJ) potential investigations of the optoelectronic properties of SnGa ₄ Q ₇ (Q=As, Se) compounds: Transparent materials for large energy conversion. Solid State Sciences, 2015, 48, 244-250.	3.2	12

#	ARTICLE	IF	CITATIONS
37	Interrelationship between structural, optical and transport properties of InP1 ⁺ Bi : DFT approach. Materials Science in Semiconductor Processing, 2016, 41, 45-53.	4.0	12
38	First-principles calculations of optoelectronic properties of CaO: Eu+2 (SrO: Eu+2) for energy applications. International Journal of Modern Physics B, 2018, 32, 1850333.	2.0	12
39	Predicted Thermoelectric Properties of the Layered XBi4S7 (X=ÅMn, Fe) Based Materials: First Principles Calculations. Journal of Electronic Materials, 2017, 46, 23-29.	2.2	11
40	Tailoring the electronic structure and optical properties of cadmium-doped zinc oxides nanosheet. Cogent Physics, 2017, 4, 1391734.	0.7	11
41	Gate dependent phonon shift in tungsten disulfide (WS ₂) field effect transistor. Materials Research Express, 2019, 6, 115909.	1.6	11
42	Density functional theory within spin-orbit coupling and hubbard correction for investigation of optoelectronic properties of the orthorhombic perovskite LaPdO3. Computational Condensed Matter, 2019, 21, e00396.	2.1	11
43	Effect of Fe doping on optoelectronic properties of CdS nanostructure: Insights from DFT calculations. Physica B: Condensed Matter, 2020, 583, 412056.	2.7	11
44	Electronic structure and related optical, thermoelectric and dynamical properties of Lilianite-type Pb7Bi4Se13: Ab-initio and Boltzmann transport theory. Materialia, 2020, 10, 100658.	2.7	11
45	Mechanical and thermodynamic stability, structural, electronics and magnetic properties of new ternary thorium-phosphide silicides ThSixP1-x: First-principles investigation and prospects for clean nuclear energy applications. Nuclear Engineering and Technology, 2021, 53, 592-602.	2.3	11
46	Study of electronic structure, charge density, Fermi energy and optical properties of Cs2KTbCl6 and Cs2KEuCl6. Physica B: Condensed Matter, 2013, 431, 102-108.	2.7	10
47	DFT combined to Boltzmann transport theory for optoelectronic and thermoelectric properties investigations for monoclinic metallic selenide: Cu5Sn2Se7. Optik, 2016, 127, 5472-5478.	2.9	10
48	Specific features of structural, electronic, optical and elastic properties of the cubic calcium pyroniobate Ca2Nb2O7 crystals. Physica B: Condensed Matter, 2018, 545, 69-75.	2.7	10
49	Structural, electronic, optoelectronic and transport properties of LuZnCuAs2 compound: First principle calculations under DFT. Physica B: Condensed Matter, 2020, 596, 412351.	2.7	10
50	An effectual enhancement to the electrical conductivity of graphene FET by silver nanoparticles. Diamond and Related Materials, 2020, 106, 107833.	3.9	10
51	Proposal of new stable <sc> ABC ₂ </sc> type ternary semiconductor pnictides <sc> K ₃ Cu ₃ P ₂ </sc> and <sc> K ₃ Ni ₃ P ₂ </sc>. International Journal of Energy Research, 2021, 45, 2980-2996.	4.5	10
52	A systematic study on optoelectronic properties of Mn⁴⁺-activated Zr-based hexafluoride red phosphors X₂ZrF₆ (X=ÅK, Na, Cs): first-principles investigation and prospects for warm-white LEDs applications. Physica Scripta, 2021, 96, 015801.	2.5	10
53	Nanosized Magnesium doped Copper Chromites Spinel Particles Synthesis and Characterization. ECS Journal of Solid State Science and Technology, 2020, 9, 126005.	1.8	10
54	Electronic structure, Fermi surface and optical properties of metallic compound Be8(B48)B2. Journal of Magnetism and Magnetic Materials, 2014, 351, 98-103.	2.3	9

#	ARTICLE	IF	CITATIONS
55	Revealing the optoelectronic properties of Re-based double perovskites using the Tran-Blaha modified Becke-Johnson with density functional theory. <i>Journal of Molecular Modeling</i> , 2020, 26, 158.	1.8	9
56	Effect of manganese on electronic and optical properties of Ba ₂ ZnS ₃ : A DFT study. <i>Journal of Solid State Chemistry</i> , 2021, 301, 122335.	2.9	9
57	Ab initio study of the structural, electronic, elastic and thermal properties of RMn ₂ Ge ₂ (R = Ca, Nd) <i>Tj ETQq1 1 0.784314 rgBT /Overlo</i>	5.5	8
58	Theoretical calculations for MUO ₃ (M = Na; K; Rb): DFT study. <i>Journal of Organometallic Chemistry</i> , 2014, 766, 22-33.	1.8	8
59	Transport properties of APdCu(Se ₂)(Se ₃) (A = K and Rb): new quaternary copper palladium polyselenides. <i>RSC Advances</i> , 2014, 4, 20102-20113.	3.6	7
60	Elastic and optoelectronic properties of novel Ag ₃ AuSe ₂ and Ag ₃ AuTe ₂ semiconductors. <i>Materials Science in Semiconductor Processing</i> , 2016, 52, 8-15.	4.0	7
61	Synthesis and Fabrication of Co _{1-x} Ni _x Cr ₂ O ₄ Chromate Nanoparticles and the Effect of Ni Concentration on Their Bandgap, Structure, and Optical Properties. <i>Journal of Composites Science</i> , 2021, 5, 247.	3.0	7
62	Electronic, optical and thermoelectric properties of Ce ₃ PdIn ₁₁ and Ce ₅ Pd ₂ In ₁₉ : An ab initio study. <i>Intermetallics</i> , 2014, 55, 184-194.	3.9	6
63	Electronic structure, effective mass, and optical dispersion of 2-mercapto-5-methyl-1,3,4-thiadiazole: density functional theory calculations. <i>Materials Science in Semiconductor Processing</i> , 2014, 26, 649-656.	4.0	6
64	Density of states, optical and thermoelectric properties of perovskite vanadium fluorides Na ₃ VF ₆ . <i>Journal of Magnetism and Magnetic Materials</i> , 2014, 358-359, 16-22.	2.3	6
65	Electronic structure and thermoelectric properties of PbS _{1-x} Tex (x=0, 0.25, 0.50, 0.75, 1.0) alloys: Ab initio study. <i>Superlattices and Microstructures</i> , 2018, 124, 248-256.	3.1	6
66	Optoelectronic Structure and Related Transport Properties of Ag ₂ Sb ₂ O ₆ and Cd ₂ Sb ₂ O ₇ . <i>Journal of Electronic Materials</i> , 2018, 47, 1481-1489.	2.2	6
67	A first-principles theoretical investigation of the structural, electronic and magnetic properties of cubic thorium carbonitrides ThC _x N _(1-x) . <i>Nuclear Engineering and Technology</i> , 2019, 51, 1373-1380.	2.3	6
68	DFT modeling of thermoelectric and optical features of novel MgxSn _{1-x} Se (x = 6%, 12% & 18%). <i>Journal of Molecular Graphics and Modelling</i> , 2020, 94, 107484.	2.4	6
69	Cation effect on electronic, optical and thermoelectric properties of perovskite oxynitrides: Density functional theory. <i>Materials Science in Semiconductor Processing</i> , 2020, 107, 104800.	4.0	6
70	Electronic structure, Fermi surface topology and spectroscopic optical properties of LaBaCo ₂ O _{5.5} compound. <i>Journal of Magnetism and Magnetic Materials</i> , 2014, 363, 133-139.	2.3	5
71	Electrical transport properties of potassium germanide tungstates (K ₁₀ Ge ₁₈ WO ₄): A theoretical study. <i>Solid State Sciences</i> , 2014, 32, 26-34.	3.2	5
72	Exploring the thermoelectric and magnetic properties of uranium selenides: Tl ₂ Ag ₂ USe ₄ and Tl ₃ Cu ₄ USe ₆ . <i>Journal of Magnetism and Magnetic Materials</i> , 2016, 413, 57-64.	2.3	5

#	ARTICLE	IF	CITATIONS
73	DFT study of optoelectronic and magnetic properties of iron-containing diamond-like materials Ag ₂ FeSiS ₄ , Li ₂ FeSnS ₄ , and Li ₂ FeGeS ₄ . Solid State Sciences, 2017, 72, 71-79.	3.2	5
74	An ab-initio investigation of the electronic structure, chemical bonding and optical properties of Ba ₂ HgS ₅ semiconductor. Molecular Physics, 2020, 118, e1587026.	1.7	5
75	Effect of Coulomb interactions on optoelectronic properties of Eu doped lanthanide stannates pyrochlore: DFT+U investigations. Journal of Solid State Chemistry, 2020, 290, 121522.	2.9	5
76	Ab-initio study of Cu-based oxychalcogenides: A new class of materials for optoelectronic applications. Journal of Solid State Chemistry, 2020, 284, 121191.	2.9	5
77	First principle approach to substitutional effect of europium (Eu ²⁺) on electronic and optical parameters of strontium pyroniobate for low temperature applications. Journal of Alloys and Compounds, 2021, 854, 157115.	5.5	5
78	Insight into the Structural, Magneto-electronic, and Mechanical Characteristic of Y ₂ MnZ (Z = Al, Ga, In) T ₁ ET ₂ O ₁₀ Orthorhombic /Overl	1.8	5
79	Thermoelectric, band structure, chemical bonding and dispersion of optical constants of new metal chalcogenides Ba ₄ CuGa ₅ Q ₁₂ (Q = S, Se). Journal of Magnetism and Magnetic Materials, 2014, 362, 204-215.	2.3	4
80	First principle study of the electronic structure, Fermi surface, electronic charge density and optical properties of ThCu ₅ In and ThCu ₅ Sn single crystals. Journal of Magnetism and Magnetic Materials, 2014, 352, 72-80.	2.3	4
81	Optoelectronic behavior of Quaternary Uranium Chalcogenides Rb ₂ Pd ₃ UM ₆ (M = S, Se): A first principle study. Journal of Alloys and Compounds, 2014, 615, 507-513.	5.5	4
82	Theoretical investigation of electronic structure and optical response in relation to the transport properties of Ga _{1-x} In _x N (x = 0, 0.25, 0.50, 0.75). Current Applied Physics, 2015, 15, 608-616.	2.4	4
83	GGA+U study on phase transition, optoelectronic and magnetic properties of AmO ₂ with spin-orbit coupling. Journal of Magnetism and Magnetic Materials, 2015, 396, 190-197.	2.3	4
84	Thermoelectric and optoelectronic properties of a heterocyclic isoxazolone nucleus compound. Materials Science in Semiconductor Processing, 2015, 30, 197-207.	4.0	4
85	Engel-Vosko GGA Approach Within DFT Investigations of the Optoelectronic Structure of the Metal Chalcogenide Semiconductor CsAgGa ₂ Se ₄ . Journal of Electronic Materials, 2016, 45, 746-754.	2.2	4
86	Polymorph phosphor SrSi ₂ O ₂ N ₂ :Eu ²⁺ optoelectronic properties for highly efficient LED: ab-initio calculations. Materials Today Communications, 2017, 13, 263-268.	1.9	4
87	Specific thermoelectric features of novel CaPd ₃ B ₄ O ₁₂ (B = Ti, V) perovskites following DFT calculations. Physica B: Condensed Matter, 2018, 545, 330-336.	2.7	4
88	Insight into the Optoelectronic and Thermoelectric Properties of Mn Doped ZnTe from First Principles Calculation. Crystals, 2019, 9, 247.	2.2	4
89	Magnetic and electrical properties of Ba ₂ Co ₂ Fe ₁₂ O ₂₂ /PANI composites prepared by insitu polymerization. Physica B: Condensed Matter, 2020, 597, 412410.	2.7	4
90	Optoelectronic properties of Nd ³⁺ doped CaTa ₂ O ₆ : Insights from the GGA+U calculations. Optik, 2021, 225, 165270.	2.9	4

#	ARTICLE	IF	CITATIONS
91	Insight into electronic and optical properties of Eu ²⁺ -doped CaTiO ₃ from GGA+U calculations. Journal of Solid State Chemistry, 2021, 293, 121796.	2.9	4
92	Rb and Cs doping effects in sodium borohydride: Density functional theory for hydrogen (H ₂) storage purpose. International Journal of Hydrogen Energy, 2021, 46, 2405-2412.	7.1	4
93	Insight view of Hf ₂ CrZ (Z = B, Ga, In, Si, Ge, Sn) Heusler materials via DFT calculations: A study on structural, electronic and magnetic properties. Computational Condensed Matter, 2021, 26, e00518.	2.1	4
94	Structural, electronic, optical and thermodynamical properties of Cu ₃ Se ₂ and [Cu ₃ Se ₂]:Zn compounds: Using DFT. Journal of Solid State Chemistry, 2021, 298, 122125.	2.9	4
95	The effect of substitutional doping of Yb ²⁺ on structural, electronic, and optical properties of CsCaX ₃ (X: Cl, Br, I) phosphors: a first-principles study. Journal of Physics Condensed Matter, 2022, 34, 065502.	1.8	4
96	Effects of Mn ²⁺ doping on the electronic, structural, and optical properties of Cs ₂ ZrF ₆ : An ab initio study. Journal of Physics and Chemistry of Solids, 2022, 162, 110492.	4.0	4
97	First principle investigation of electronic structure, chemical bonding and optical properties of tetrabarium gallium trinitride oxide single crystal. Materials Research Bulletin, 2015, 70, 436-441.	5.2	3
98	Structural, elastic, optoelectronic and magnetic properties of CdHo_2S_4 spinel: a first-principle study. Bulletin of Materials Science, 2017, 40, 1105-1110.	1.7	3
99	Spin Gapless Semiconductor to Nonmagnetic Semiconductor Transitions in Fe-Doped Ti ₂ CoSi: First-Principle Calculations. Applied Sciences (Switzerland), 2018, 8, 2200.	2.5	3
100	DFT simulations of optoelectronic and elastic features of cubic samarium zirconate (Sm ₂ Zr ₂ O ₇). Computational Condensed Matter, 2019, 21, e00414.	2.1	3
101	Study of electrical attributes of molybdenum ditelluride (MoTe ₂) FET using experimental and theoretical evidences. Microelectronic Engineering, 2020, 230, 111365.	2.4	3
102	Exploring the potential use of Ca[LiAl ₃ N ₄]:Eu ²⁺ as phosphor-LED material: Ab-initio calculations. Materials Today Communications, 2020, 25, 101302.	1.9	3
103	On the role of Zn doping on tuning the electronic and optical properties of MnCr ₂ O ₄ spinel via Mn _{0.5} Zn _{0.5} Cr ₂ O ₄ doping scheme: A first-principles quantum computational analysis. Physica Scripta, 2022, 97, 045812.	2.5	3
104	Optoelectronic features of NbCu ₃ Q ₄ (Q = S, Se) for p-type transparent conducting application: DFT and HSE06. Optik, 2022, 262, 169297.	2.9	3
105	Density functional theory-based quantum-computational analysis on the strain-assisted phononic, electronic, photocatalytic properties and thermoelectric performance of monolayer Janus SnSse. Applied Physics A: Materials Science and Processing, 2022, 128, .	2.3	3
106	The electronic structure, electronic charge density and optical properties of the diamond-like semiconductor Ag ₂ ZnSi ₄ . Applied Physics A: Materials Science and Processing, 2014, 116, 333-340.	2.3	2
107	Thermoelectric properties of quaternary Uranium chalcogenides Cs ₂ Pt ₃ US ₆ and Cs ₂ Pt ₃ USe ₆ . Solid State Sciences, 2014, 34, 56-62.	3.2	2
108	Exploring the optoelectronic properties of Nitrido-magneso-silicates: Ca[Mg ₃ SiN ₄], Sr[Mg ₃ SiN ₄], and Eu[Mg ₃ SiN ₄]. Semiconductor Science and Technology, 2017, 32, 055017.	2.0	2

#	ARTICLE	IF	CITATIONS
109	A comparative study of structural, electronic and magnetic properties of DyOCl and HoOCl lanthanide oxychlorides: first-principles predictions of DFT, DFT + U and DFT + U + SOC methods. Materials Research Express, 2019, 6, 126129.	1.6	2
110	Electronic, elastic, thermodynamic and vibrational properties of Li ₆ BeZrF ₁₂ : Insights from DFT-based computer simulation. Computational Condensed Matter, 2020, 25, e00506.	2.1	2
111	Exploring fundamental properties of Mg _{0.915} Al _{0.085} H ₂ (A = Ti, Fe) for potential hydrogen storage application: First-principles study. International Journal of Energy Research, 2021, 45, 14971-14984.	4.5	2
112	Electronic band structure and optical characteristic of silver lanthanide XAgSe ₂ (X = Eu and Er) dichalcogenides: Insight from DFT computations. Inorganic Chemistry Communication, 2021, 129, 108586.	3.9	2
113	Electronic structure, chemical bonding and optical properties of Di-2-pyrimidonium dichloride diiodide (C ₄ H ₅ Cl ₂ N ₂ O) from first-principles. Materials Science in Semiconductor Processing, 2015, 31, 372-379.	4.0	1
114	Density Functional Theory Investigations of the Optoelectronic Properties of Li ₂ MnGeS ₄ and Li ₂ CoSnS ₄ . Spin, 2019, 09, 1950015.	1.3	1
115	Proposal of new spinel oxides semiconductors ZnGaO ₂ , [ZnGaO ₂]:Mn ³⁺ and Rh ³⁺ : ab-initio calculations and prospects for thermophysical and optoelectronic applications. Journal of Molecular Graphics and Modelling, 2020, 101, 107750.	2.4	1
116	A first-principles investigation on electronic, optical and thermoelectric properties of $\text{La}_2\text{Pd}_2\text{O}_5$ compound. Bulletin of Materials Science, 2020, 43, 1.	1.7	1
117	Optoelectronic investigation of lithium di-manganese oxide with doping of Nickel via Li _{1-x} Ni _x Mn ₂ O ₄ where X= 4 % and 8% composition and their application. Journal of Solid State Chemistry, 2022, 309, 122918.	2.9	1
118	Theoretical study of the new zintl phases compounds K ₂ ACdSb ₂ (A=(Sr, Ba)). Physica B: Condensed Matter, 2015, 464, 9-16.	2.7	0
119	Optoelectronic and Magnetic Properties of Eu ₂ Si ₅ N ₈ : An Ab-initio Study. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2015, 70, 897-904.	1.5	0
120	First-principles investigation of the electronic band structures and optical properties of quaternary BaM_4Q ($\text{A} = \text{Rb, Cs}$; $\text{M} = \text{P, V}$; and $\text{Q} = \text{S}$) metal chalcogenides. International Journal of Modern Physics B, 2018, 32, 1850337.	2.0	0
121	Effect of pressure and Hubbard potential on the electronic and magnetic properties of thorium monpnictides ThPn (Pn = N, P, As, Sb, Bi) in respect of crystal field splitting, charge transfer and spin flipping of magnetic moments. Computational Condensed Matter, 2019, 21, e00403.	2.1	0