Åule UÇ§ur

List of Publications by Year
in descending order

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106	1,144	430442	552369
papers	citations	18 h-index	26 g-index

107	107	107	796
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Prediction of the electronic structure, optical and vibrational properties of ScXCo2Sb2 (Xâ€‰=â€‰V, Nb and) Tj ETQq1 1 0.784314 rg	0.9	3
2	Electronic, elastic, mechanical and anisotropic response of W3XC2 (X: Si, Ge and Al) alloys via first-principles. Solid State Communications, 2022, 343, 114648.	0.9	2
3	Chemical bonding, magnetic and electronic properties, mechanical and dynamical stabilities of DyOs4P12 filled-skutterudite: DFT and QTAIM insight. Materials Chemistry and Physics, 2022, 278, 125684.	2.0	1
4	Investigating the Magnetic, Mechanical, Electronic, Optical, and Anisotropic Properties of ZrCoFeX (Xâ€‰=â€‰Si, Ge) Quaternary Heusler Alloys via First Principles. Journal of Superconductivity and Novel Magnetism, 2022, 35, 1173-1182.	0.8	5
5	First-principles calculations of electronic and optical properties of AgGa1-xTlxS2 alloys: Analyses and design for solar cell applications. Journal of Solid State Chemistry, 2022, 309, 122996.	1.4	4
6	Exploring the elastic, mechanical and anisotropic response of Ti-5Al-XSn alloys through DFT calculations. Chinese Journal of Physics, 2022, 77, 151-160.	2.0	7
7	Dynamical and mechanical stability, electronic properties, bonding and weak interactions analysis of new compounds MgS2 and MgSe2 in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mrow><mml:mtext>Pa</mml:mtext><mml:mover accent="true"><mml:mn>3</mml:mn><mml:mo stretchy="true">â€¾</mml:mo></mml:mover></mml:mrow></mml:math> space group structure: Ab initio study. Materials Science in Semiconductor Processing, 2022, 146, 106659.	1.9	12
8	The elastic, mechanical, and thermodynamic properties of NaXH (X = B, Al) intended for the storage of hydrogen: An ab-initio study. Physica B: Condensed Matter, 2022, 638, 413851.	1.3	3
9	Analyzing the electronic and optical properties of bulk, unstrained, and strained monolayers of SrS2 by DFT. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 143, 115403.	1.3	4
10	Elastic isotropy, magnetic and electronic properties, bonding and non-covalent interactions analyses of HoFe4P12 filled-skutterudite: DFTÂ+ÂUÂ+ÂSOC, QTAIM and NCI investigations. Journal of Magnetism and Magnetic Materials, 2021, 518, 167435.	1.0	4
11	Elastic, mechanical, optical and magnetic properties of Ru2MnX (XÂ=ÂNb, Ta, V) Heusler alloys. Journal of Magnetism and Magnetic Materials, 2021, 523, 167614.	1.0	24
12	Electronic structure, optical and vibrational properties of Ti2FeNiSb2 and Ti2Ni2InSb double half heusler alloys. Materials Science in Semiconductor Processing, 2021, 123, 105531.	1.9	18
13	Elastic, mechanical, anisotropic, optical and magnetic properties of V₂NiSb Heusler alloy. Physica Scripta, 2021, 96, 035807.	1.2	9
14	First principles study of electronic, elastic, optical and magnetic properties of Rh 2 MnX (X = Ti, Hf, Sc,) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.0	14
15	Structural, elastic and mechanical properties of Tiâ€“15Nbâ€“xGe alloys: insight from DFT calculations. Bulletin of Materials Science, 2021, 44, 1.	0.8	6
16	First principles study of structural, elastic, mechanical and electronic properties of nitrogen-doped cubic diamond. Bulletin of Materials Science, 2021, 44, 1.	0.8	29
17	A comparative study of structural, thermal, and optoelectronic properties between zircon and scheelite type structures in SrMoO4 compound: An ab-initio study. Optik, 2021, 238, 166714.	1.4	5
18	A first-principles study for the elastic and mechanical properties of Ti64, Ti6242 and Ti6246 alloys. European Physical Journal B, 2021, 94, 1.	0.6	6

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19	An ab-initio investigation of the electronic structure, chemical bonding and optical properties of Ba₂HgS₅ semiconductor. Molecular Physics, 2020, 118, e1587026.	0.8	5
20	First principles study of elastic and mechanical properties of TlBr and TlCl compounds. Journal of Molecular Structure, 2020, 1200, 127150.	1.8	11
21	Study of the ground-state magnetic ordering, magnetic and optoelectronic properties of (Lenaite) AgFeS2 in its chalcopyrite structure. Journal of Magnetism and Magnetic Materials, 2020, 493, 165730.	1.0	18
22	DFT-investigation on anisotropy degree of electronic, optical, and mechanical properties of olivine ZnRE2S4 (RE = Er, Tm) compounds. Materials Research Express, 2020, 7, 016305.	0.8	3
23	Insight into the role of weak interactions on optoelectronic properties of LiGaTe2-chalcopyrite under pressure effect: DFT-D3, NCI and QTAIM investigations. Physica B: Condensed Matter, 2020, 599, 412463.	1.3	15
24	Ab Initio Full-Potential Study of the Structural, Electronic, and Magnetic Properties of the Cubic Sr0.75Ti0.25X (X = S, Se, and Te) Ternary Alloys. Journal of Superconductivity and Novel Magnetism, 2020, 33, 3263-3272.	0.8	7
25	First principles investigations of structural, elastic, mechanical, electronic and optical properties of triple perovskite Ba2K2Te2O9. Physica B: Condensed Matter, 2020, 596, 412404.	1.3	10
26	Study of structural, elastic, electronic, and vibrational properties of MRh2O4 (M = Cd and Zn) spinels: DFT-based calculations. Journal of Molecular Modeling, 2020, 26, 140.	0.8	2
27	A theoretical study for the band gap energies of the most common silica polymorphs. Chinese Journal of Physics, 2020, 65, 472-480.	2.0	21
28	Pressure induced phase transition, electronic and optical properties of LiBeX (X = As, Sb and Bi). Journal of Physics Condensed Matter, 2020, 32, 325503.	0.7	4
29	Cation distribution effect on electronic, magnetic structure and optic properties in cobalt ferrites (Co _{1â^'y} Fe _y)_{Tet}(Co) Tj ETQq1 1 0.784314 rgBT /C with disordered spinel structure. Physica Scripta, 2020, 95, 105801.	1.2	4
30	Structural, elastic, electronic and vibrational properties of XAl2O4 (XÂ=ÂCa, Sr and Cd) semiconductors with orthorhombic structure. Journal of Alloys and Compounds, 2019, 809, 151773.	2.8	9
31	Phase transitions and lattice dynamics in perovskite-type hydride $oldsymbol{{m Li}_{x} {m Na}_{1-x} {m MgH}_{3}}$. Journal of Physics Condensed Matter, 2019, 31, 505402.	0.7	2
32	Pressure effect on mechanical stability and ground state optoelectronic properties of Li2S2 produced by Lithiumâ^'Sulfur batteries discharge: GGA-PBE, GLLB-SC and mBJ investigation. Philosophical Magazine, 2019, 99, 2789-2817.	0.7	1
33	First principles investigations of the structural, elastic, vibrational, and thermodynamic properties of TiMg2O4 oxide spinels: cubic and tetragonal phases. Journal of Molecular Modeling, 2019, 25, 210.	0.8	1
34	Structural, elastic, electronic and thermoelectric properties of XPN₂ (X =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.0	11
35	First Brillouin zone-centre phonon frequencies and elastic stiffness of the Ln2Hf2O7 (LnÂ= La, Nd, Sm) Tj ETQq1 1 0.784314 rgBT /Ov	0.9	1
36	Lattice dynamical and elastic properties of BaFX(X= Cl, Br and I): Matlockite structure compounds. International Journal of Modern Physics B, 2019, 33, 1950221.	1.0	4

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37	Structural, electronic, optical and elastic properties of XLa2S4 (Xâ€¯=â€¯Ba; Ca): Ab initio study. Physica B: Condensed Matter, 2019, 558, 91-99.	1.3	10
38	Insight into the structural, elastic, electronic, thermoelectric, thermodynamic and optical properties of MRhSb (Mâ€¯=â€¯Ti, Zr, Hf) half-Heuslers from ab initio calculations. Chinese Journal of Physics, 2019, 59, 434-448.	2.0	17
39	First principles investigations of the structural, elastic, electronic, vibrational and thermodynamic properties of hexagonal XAl₂O₄ (X = Cd, Ca and Sr). Materials Research Express, 2019, 6, 085518.	0.8	2
40	Basis set convergence of binding energy with and without CP-correction utilizing PBE0 method: A benchmark study of X2 (X=Ge, As, Se, Sc, Ti, V, Cr, Mn, Co, Cu, Zn). Journal of Theoretical and Computational Chemistry, 2019, 18, 1950034.	1.8	0
41	Theoretical research on structural, electronic, mechanical, lattice dynamical and thermodynamic properties of layered ternary nitrides Ti2AN (Aâ€¯=â€¯Si, Ge and Sn). Journal of Alloys and Compounds, 2019, 771, 664-673.	2.8	34
42	Electronic structure and magnetic properties of manganese-based MnAs1âˆ’xPx ternary alloys. Journal of Magnetism and Magnetic Materials, 2019, 469, 329-341.	1.0	3
43	Effect of Structure on the Electronic, Magnetic and Thermal Properties of Cubic Fe2MnxNi1âˆ’xSi Heusler Alloys. Journal of Electronic Materials, 2019, 48, 337-351.	1.0	5
44	First-principle calculations of structural, electronic and magnetic investigations of Mn2RuGe1-xSnx quaternary Heusler alloys. Chinese Journal of Physics, 2018, 56, 567-573.	2.0	72
45	Structural, electronic, elastic, optical and vibrational properties of MAl2O4 (M = Co and Mn) aluminate spinels. Ceramics International, 2018, 44, 310-316.	2.3	17
46	External pressure effect on the electronic, optical and thermoelectric properties of the CdY2Ch4 (Ch) Tj ETQq0 0 0 rgBT /Overlock 10 Tf Matter, 2018, 545, 40-47.	1.3	9
47	Investigation of structural, elastic, electronic, optical and vibrational properties of silver chromate spinels: Normal (CrAg2O4) and inverse (Ag2CrO4). Journal of Alloys and Compounds, 2017, 704, 101-108.	2.8	26
48	Electronic structure, phase stability, vibrational and thermodynamic properties of the ternary Nowotny-Juza materials LiMgSb and LiZnSb. Physica B: Condensed Matter, 2017, 519, 39-52.	1.3	7
49	Ab-Initio Calculations and Thermodynamic Description of the Yb-Cd and Yb-Sn Systems. Journal of Phase Equilibria and Diffusion, 2017, 38, 665-675.	0.5	0
50	Investigation of the structural, electronic, elastic and thermodynamic properties of Curium Monopnictides: An abÂinitio study. International Journal of Modern Physics B, 2017, 31, 1750226.	1.0	5
51	First-principles investigation of superconductivity in the body-centred tetragonal. Philosophical Magazine, 2016, 96, 2059-2073.	0.7	11
52	Optoelectronic and thermoelectric properties of Zintl YLi ₃ A ₂ () Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 107801.	0.7	5
53	A first-principle study of Os-based compounds: Electronic structure and vibrational properties. Journal of Physics and Chemistry of Solids, 2016, 96-97, 121-127.	1.9	17
54	Electron-phonon superconductivity in the ternary phosphides<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ba</mml:mi><mml:msub><mml:mi>M</mml:mi><mml:m mathvariant="normal">P</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math><mml:math		

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55	Theoretical investigation of superconductivity in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>SrPd</mml:mi><mml:mn>2</mml:mn></ xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>SrPd</mml:mi><mml:mn>2</mml:mn></ and<mml:math xmlns:mml="http://www.w3.org/1998. Physical Review B, 2016, 93, .	1.1	10
56	Investigation of electronic structure and thermodynamic properties of quaternary Li-containing chalcogenide diamond-like semiconductors. Semiconductor Science and Technology, 2016, 31, 125015.	1.0	1
57	Structural, electronic, optical and elastic properties of the complex K₂PtCl₆-structure hydridesARuH₆(A= Mg, Ca, Sr and) Tj ETQq1 1 0.784314 rgBT	1.7	37
58	Electronic structure, optical and thermodynamic properties of ternary hydridesMBeH₃(M= Li, Na, and K). Canadian Journal of Physics, 2016, 94, 865-876.	0.4	8
59	First principles study of hydrogen storage material NaBH₄and LiAlH₄compounds: electronic structure and optical properties. Physica Scripta, 2016, 91, 045804.	1.2	24
60	Ab initioinvestigation of BCS-type superconductivity in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">LuNi</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">C</mml:mi></mml:math>-type superconductors. Physical Review B, 2015, 92, .	1.1	33
61	Identification of specific phonon contributions in BCS-type superconductivity of boride-carbide crystals with a layer-like structure. Solid State Communications, 2015, 206, 1-5.	0.9	3
62	Structural, elastic, electronic, phonon and thermal properties of Ir₃Ta and Rh₃Ta alloys. Philosophical Magazine Letters, 2015, 95, 392-400.	0.5	7
63	Thermodynamic description of the Biâ€“Cs and Biâ€“Tm system supported by first-principles calculations. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2015, 48, 72-78.	0.7	10
64	Structural phase transition and opto-electronic properties of NaZnAs. Journal of Alloys and Compounds, 2015, 622, 812-818.	2.8	1
65	Electronic structure, phase stability, and vibrational properties of Ir-based intermetallic compound IrX (X=Al, Sc, and Ga). Journal of Physics and Chemistry of Solids, 2015, 77, 126-132.	1.9	22
66	First-Principles Calculations and Thermodynamic Assessment of the Li-Rh and Tl-Tm Systems. International Journal of Materials Mechanics and Manufacturing, 2015, 4, 135-139.	0.2	0
67	Preface of the â€œSymposium on first-principles investigation of structural, electronic, elastic, thermodynamic and phonon properties of materialsâ€, , 2014, , .		0
68	Calculations of structural, elastic, electronic, magnetic and phonon properties of FeNiMnAl by the first principles. , 2014, , .		1
69	Structural, elastic, electronic, magnetic and vibrational properties of CuCoMnGa under pressure. AIP Conference Proceedings, 2014, , .	0.3	1
70	Elastic and phonon properties of quaternary Heusler alloys CoFeCrZ (Z = Al, Si, Ga and Ge) from density functional theory. Philosophical Magazine Letters, 2014, 94, 708-715.	0.5	25
71	Electronic and phonon properties of the full-Heusler alloys X2YAl (XÂ=ÂCo, Fe and YÂ=ÂCr, Sc): a density functional theory study. Journal of Materials Science, 2014, 49, 4180-4190.	1.7	42
72	Phase transition of Nowotnyâ€“Juza NaZnX (X=P, As and Sb) compounds at high pressure: Theoretical investigation of structural, electronic and vibrational properties. Computational Materials Science, 2014, 87, 187-197.	1.4	23

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73	Ab-initio study of the structural, electronic, elastic and vibrational properties of the intermetallic Pd3V and Pt3V alloys in the L12 phase. Metals and Materials International, 2014, 20, 765-773.	1.8	11
74	Structural, elastic, electronic, chemical bonding and optical properties of Cu-based oxides ACuO (A=Li, Na, K and Rb): An ab initio study. Computational Materials Science, 2014, 81, 561-574.	1.4	53
75	Ab initio study of structural, electronic, magnetic and optical properties of Ti-doped ZnTe and CdTe. International Journal of Modern Physics B, 2014, 28, 1450080.	1.0	12
76	Elastic and thermodynamic properties of ZnSc2S4 and CdSc2S4 compounds under pressure and temperature effects. Computational Materials Science, 2013, 70, 107-113.	1.4	18
77	Structural, elastic, electronic and phonon properties of scandium-based compounds ScX3 (X=Ir, Pd, Pt) Tj ETQq1 1 0.784314 rgBT /Ov	1.4	23
78	Prediction Study of the Mechanical and Thermodynamic Properties of the $$hbox {RBRh}_{3}$$ RBRh 3 (R $$=$$ = Sm, Eu, Gd, and Tb) Compounds. International Journal of Thermophysics, 2013, 34, 2102-2118.	1.0	0
79	A first-principles study of the structural, elastic, electronic and phonon properties of LiMgP and LiMgAs in the Î±, Î² and Î³ phases. Journal of Alloys and Compounds, 2013, 551, 108-117.	2.8	5
80	Structural, electronic and vibrational properties of ordered intermetallic alloys CoZ (Zâ€‰=â€‰Al, Be, Sc) Tj ETQq0 0 0 rgBT /Overlock	0.7	11
81	Structural, Elastic, Electronic and Optical Properties of Cu₃TMSe₄ (TM = V,) Tj ETQq1 1 0.784314 rgBT /Ov 5, 97-106.	0.1	29
82	AB INITIO STUDY OF PHONON DISPERSION AND ELASTIC PROPERTIES OF L1₂ INTERMETALLICS Ti₃Al AND Y₃Al. Modern Physics Letters B, 2013, 27, 1350224.	1.0	4
83	First-principles study of B2-like intermetallics LaMg and YMg. Intermetallics, 2012, 22, 218-225.	1.8	4
84	Theory study of structural parameters, elastic stiffness, electronic structures and lattice dynamics of RBRh3 (R=Sc, Y, La and Lu). Computational Materials Science, 2012, 54, 336-344.	1.4	4
85	Ab initio study of some fundamental physical properties of the cubic inverse-perovskite Mn3ZnC and Mn3GeC. Computational Materials Science, 2012, 58, 162-166.	1.4	5
86	DFT-BASEDAB INITIOSTUDY OF THE ELECTRONIC AND OPTICAL PROPERTIES OF CESIUM BASED FLUORO-PEROVSKITECsMF₃(M = CaANDSr). International Journal of Modern Physics B, 2012, 26, 1250199.	1.0	18
87	Full-Potential Calculation of Structural, Electronic, and Thermodynamic Properties of Fluoroperovskite $$ext{ CsMF}_{3}$$ (MÂ=ÂBe and Mg). International Journal of Thermophysics, 2012, 33, 2339-2350.	1.0	2
88	Electronic and phonon properties of Sc-TM (TM=Ag, Cu, Pd, Rh, Ru) compounds. Computational Materials Science, 2010, 47, 668-671.	1.4	15
89	Phonon and elastic properties of AlSc and MgSc from first-principles calculations. Computational Materials Science, 2010, 48, 866-870.	1.4	33
90	Structural, electronic and phonon properties of MoTa and MoNb: a density functional investigation. Physica Scripta, 2010, 82, 015601.	1.2	1

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91	Theoretical study of the phonon properties of SrS. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2009, 162, 116-119.	1.7	21
92	Structural, electronic and elastic properties of YCu from first principles. Journal of Rare Earths, 2009, 27, 661-663.	2.5	10
93	Electronic structure calculations of rare-earth intermetallic compound YAg using ab initio methods. Journal of Rare Earths, 2009, 27, 664-666.	2.5	13
94	Structural, electronic and phonon propertiesâ€™ investigation of YP and YAs compounds. Journal of Physics and Chemistry of Solids, 2008, 69, 791-798.	1.9	21
95	First principles linear response calculations of phonons for ScP and ScAs. Solid State Communications, 2008, 147, 198-200.	0.9	11
96	STRUCTURAL, ELECTRONIC AND PHONON PROPERTIES OF LaX COMPOUNDS (X = P, As). International Journal of Modern Physics B, 2008, 22, 5027-5033.	1.0	6
97	Structural, Electronic and Dynamical Properties of GeSi: An Ab-initio Study. AIP Conference Proceedings, 2007, , .	0.3	0
98	Ab-initio Study of Electronic Structure of ScAuSn. AIP Conference Proceedings, 2007, , .	0.3	0
99	First-Principle Calculations of Electronic and Dynamical Properties of GeSn. AIP Conference Proceedings, 2007, , .	0.3	0
100	First-principles investigation of structural, electronic and dynamical properties in ScAuSn alloy. Computational Materials Science, 2007, 41, 134-137.	1.4	1
101	Energy/power breakdown of pipelined nanometer caches (90nm/65nm/45nm/32nm). , 2006, , .		30
102	First-principles study of surface phonons on the AlN(110) surface. Surface Science, 2004, 566-568, 904-908.	0.8	2
103	Phonon Dispersion of Fe-30%Mn Alloy. Physica Scripta, 1999, 60, 569-571.	1.2	1
104	First principles study of the electronic, optical, elastic and thermoelectric properties of Nb2WNi alloy. Molecular Physics, 0, , e1928314.	0.8	8
105	DFT aspects of the elastic, mechanical, magnetic, thermodynamic and optical properties of Ce3XY perovskites. Philosophical Magazine, 0, , 1-20.	0.7	7
106	Probing the electronic, elastic, mechanical and anisotropic features of ZrTiX(4) alloys via density functional theory. Europhysics Letters, 0, , .	0.7	0