GÃ¶kay UÄur

List of Publications by Year
in descending order

109 papers	1,085 citations	471371 17 h-index	526166 27 g-index
111 all docs	111 docs citations	111 times ranked	745 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	Structural, elastic and mechanical properties of Hf-doped TiAl2 and Î±-TiAl3 intermetallic compounds: first-principle calculations. European Physical Journal B, 2022, 95, .	0.6	5
10	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
11	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
12	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
13	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
14	Elastic, mechanical, anisotropic, optical and magnetic properties of V₂NiSb Heusler alloy. Physica Scripta, 2021, 96, 035807.	1.2	9
15	First principles study of electronic, elastic, optical and magnetic properties of Rh 2 MnX (X = Ti, Hf, Sc,) Tj ETQq1 1 0.784314 rgBT /Ov	1.0	14
16	Structural, elastic and mechanical properties of Tiâ€“15Nbâ€“xGe alloys: insight from DFT calculations. Bulletin of Materials Science, 2021, 44, 1.	0.8	6
17	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
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	First principles study of elastic and mechanical properties of TlBr and TlCl compounds. Journal of Molecular Structure, 2020, 1200, 127150.	1.8	11
20	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
21	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
22	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
23	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
24	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
25	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
26	Cation distribution effect on electronic, magnetic structure and optic properties in cobalt ferrites (Co _{1â^'y} Fe _y)_{Tet}(Co) Tj ETQq0 0 0 rgBT /Overlock with disordered spinel structure. Physica Scripta, 2020, 95, 105801.	1.2	4
27	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
28	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
29	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
30	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
31	Structural, elastic, electronic and thermoelectric properties of XPN₂ (X =) Tj ETQq1 1 0.784314 rgBT /Over	1.0	11
32	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
33	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
34	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
35	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
36	Thermodynamic Modeling of the Al-Ba and Ba-Ge Systems Supported by First-Principles Calculations. Journal of Phase Equilibria and Diffusion, 2019, 40, 195-205.	0.5	3

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37	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
38	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
39	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
40	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
41	Insight into the optoelectronic and thermoelectric properties of Ca-based Zintl phase CaCd 2 X 2 (X =) Tj ETQq1 1 0.784314 rgBT /Overl	1.3	6
42	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
43	The effect of martensitic phase transition from cubic to tetragonal on the physical properties of V 3 Si superconductor. Intermetallics, 2018, 96, 25-32.	1.8	5
44	Structural, electronic, elastic, optical and vibrational properties of MAl2O4 (M = Co and Mn) aluminate spinels. Ceramics International, 2018, 44, 310-316.	2.3	17
45	Electronic, mechanical, and optical properties of Ruddlesden-Popper perovskite sulfides: First principle calculation. Ferroelectrics, 2018, 535, 142-151.	0.3	2
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	Band Structure and Optical Properties of Kesterite Type Compounds: first principle calculations. IOP Conference Series: Materials Science and Engineering, 2017, 175, 012014.	0.3	1
48	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
49	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
50	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
51	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
52	Computational investigations on band structure and electronic features of chromium-based carbides and nitride Cr3PX (XÂ=ÂC and N) through the FP-APW+LO approach. Superlattices and Microstructures, 2017, 109, 1-12.	1.4	10
53	Optoelectronic and thermoelectric properties of Zintl YLi ₃ A ₂ () Tj ETQq1 1 0.784314 rgBT /Overlock 107801.	0.7	5
54	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

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55	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
56	Elastic and mechanical properties of Mg3Rh intermetallic compound: An ab initio study. Journal of Magnesium and Alloys, 2016, 4, 123-127.	5.5	6
57	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
58	First principles study of hydrogen storage material NaBH₄and LiAlH₄compounds: electronic structure and optical properties. Physica Scripta, 2016, 91, 045804.	1.2	24
59	First-principles study of structural, electronic, elastic and phonon properties of AB2O4(A = Ge,Si;B =) Tj ETQq1 1 0.784314 rgBT /Over	1.0	9
60	Structural, elastic, electronic, phonon and thermal properties of Ir₃Ta and Rh₃Ta alloys. Philosophical Magazine Letters, 2015, 95, 392-400.	0.5	7
61	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
62	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
63	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
64	Preface of the â€œSymposium on first-principles investigation of structural, electronic, elastic, thermodynamic and phonon properties of materialsâ€•, 2014, , .		0
65	First principles study of the structural, elastic, electronic and phonon properties of CdX2O4 (X=Al,) Tj ETQq1 1 0.784314 rgBT /Overlo	3	
66	Structural, elastic, electronic and phonon properties of SnX2O4 (X=Mg, Zn, Cd) spinel from density functional theory. AIP Conference Proceedings, 2014, , .	0.3	0
67	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
68	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
69	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
70	Elastic and thermodynamic properties of ZnSc2S4 and CdSc2S4 compounds under pressure and temperature effects. Computational Materials Science, 2013, 70, 107-113.	1.4	18
71	Structural, elastic, electronic and phonon properties of scandium-based compounds ScX3 (X=Ir, Pd, Pt) Tj ETQq1 1 0.784314 rgBT /Ov	1.4	28
72	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

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73	Electronic structure and vibrational properties in cobalt-based full-Heusler compounds: A first principle study of Co2MnX (X=Si, Ge, Al, Ga). Journal of Alloys and Compounds, 2013, 560, 215-222.	2.8	92
74	Structural, Elastic, Electronic and Optical Properties of Cu₃TMSe₄ (TM = V,) Tj ETQq0 0 0 rgBT /Overlock 10 T 5, 97-106.	0.1	29
75	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
76	First-principles study of B2-like intermetallics LaMg and YMg. Intermetallics, 2012, 22, 218-225.	1.8	4
77	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
78	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
79	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
80	Ground state and phonon spectrum of NiSi2. Philosophical Magazine, 2011, 91, 468-476.	0.7	4
81	Phonon and elastic properties of AlSc and MgSc from first-principles calculations. Computational Materials Science, 2010, 48, 866-870.	1.4	33
82	Structural, electronic and phonon properties of MoTa and MoNb: a density functional investigation. Physica Scripta, 2010, 82, 015601.	1.2	1
83	Structural, electronic and elastic properties of YCu from first principles. Journal of Rare Earths, 2009, 27, 661-663.	2.5	10
84	Electronic structure calculations of rare-earth intermetallic compound YAg using ab initio methods. Journal of Rare Earths, 2009, 27, 664-666.	2.5	13
85	STRUCTURAL, ELECTRONIC AND PHONON PROPERTIES OF LaX COMPOUNDS (X = P, As). International Journal of Modern Physics B, 2008, 22, 5027-5033.	1.0	6
86	Structural, Electronic and Dynamical Properties of GeSi: An Ab-initio Study. AIP Conference Proceedings, 2007, , .	0.3	0
87	Ab-initio Study of Electronic Structure of ScAuSn. AIP Conference Proceedings, 2007, , .	0.3	0
88	First-Principle Calculations of Electronic and Dynamical Properties of GeSn. AIP Conference Proceedings, 2007, , .	0.3	0
89	First-principles investigation of structural, electronic and dynamical properties in ScAuSn alloy. Computational Materials Science, 2007, 41, 134-137.	1.4	1
90	Ab initio study of structural, electronic and dynamical properties of MgAuSn. European Physical Journal B, 2007, 58, 319-322.	0.6	0

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91	Ab initio calculation of the structural and dynamical properties of the zinc-blende BN and its (110) surface. Diamond and Related Materials, 2006, 15, 1161-1165.	1.8	7
92	Electronic and phonon structures of AuGa2and AuIn2. Journal of Physics Condensed Matter, 2006, 18, 6777-6784.	0.7	9
93	Theoretical study of the structural, electronic and dynamical properties of rocksalt ScN and GaN. Diamond and Related Materials, 2006, 15, 1175-1178.	1.8	22
94	Ab initiocalculation of the ground-state properties of CoSi2. Journal of Physics Condensed Matter, 2005, 17, 7127-7132.	0.7	7
95	Structural and dynamical properties of zinc-blende GaN, AlN, BN, and their (110) surfaces. Physical Review B, 2005, 71, .	1.1	49
96	First-principles study of electronic and dynamical properties of AuAl2. Physica Status Solidi C: Current Topics in Solid State Physics, 2004, 1, 3027-3030.	0.8	10
97	Vibrational properties of the Sb:InP() surface. Surface Science, 2002, 507-510, 1-6.	0.8	1
98	Elastic properties of antiferromagnetic Fe-40%Mn alloy. Journal of Materials Science Letters, 2000, 19, 127-129.	0.5	0
99	Phonon Dispersion of Fe-30%Mn Alloy. Physica Scripta, 1999, 60, 569-571.	1.2	1
100	The Lattice Dynamics of Ni-24%Fe Alloy Based on an Empirical Many-Body Potential. Acta Physica Polonica A, 1999, 96, 391-398.	0.2	0
101	The lattice dynamics of some type-I and type-II alloys. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1998, 20, 1863-1870.	0.4	2
102	Three-body effect on the lattice dynamics of Fe-28%Pd alloy. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1997, 19, 779-786.	0.4	2
103	Three-body effect on the lattice dynamics of some fcc d-band metals. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1997, 19, 787-796.	0.4	2
104	Three-body effect on the lattice dynamics of Pdâ€“10% Fe alloys. Physical Review B, 1995, 51, 3458-3461.	1.1	8
105	First principles study of the electronic, optical, elastic and thermoelectric properties of Nb2WNi alloy. Molecular Physics, 0, , e1928314.	0.8	8
106	Analytical Investigation of Maximum Stresses According to the (hkl) Layers at Stable Condition for Al-Sc Alloys. El-Cezeri Journal of Science and Engineering, 0, , .	0.1	1
107	Investigation of Elastic Anisotropy Pressure Change in Al-Sc Alloys. El-Cezeri Journal of Science and Engineering, 0, , .	0.1	0
108	DFT aspects of the elastic, mechanical, magnetic, thermodynamic and optical properties of Ce3XY perovskites. Philosophical Magazine, 0, , 1-20.	0.7	7

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109	Probing the electronic, elastic, mechanical and anisotropic features of ZrTiX(4) alloys via density functional theory. Europhysics Letters, 0, , .	0.7	0