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	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
2	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
3	Structural and dynamical properties of zinc-blende GaN, AlN, BN, and their (110) surfaces. Physical Review B, 2005, 71, .	1.1	49
4	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
5	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
6	Phonon and elastic properties of AlSc and MgSc from first-principles calculations. Computational Materials Science, 2010, 48, 866-870.	1.4	33
7	Structural, Elastic, Electronic and Optical Properties of Cu₃TMSe₄ (TM = V,) Tj ETQq1 1 0.784314 rgBT /Ov 5, 97-106.	0.1	29
8	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
9	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
10	First principles study of hydrogen storage material NaBH₄and LiAlH₄compounds: electronic structure and optical properties. Physica Scripta, 2016, 91, 045804.	1.2	24
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	Structural, elastic, electronic and phonon properties of scandium-based compounds ScX3 (X=Ir, Pd, Pt) Tj ETQq0 0 0 rgBT /Overlock 10	1.4	23
13	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
14	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
15	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
16	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
17	Elastic and thermodynamic properties of ZnSc2S4 and CdSc2S4 compounds under pressure and temperature effects. Computational Materials Science, 2013, 70, 107-113.	1.4	18
18	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

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19	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
20	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
21	Structural, electronic, elastic, optical and vibrational properties of MAl2O4 (M = Co and Mn) aluminate spinels. Ceramics International, 2018, 44, 310-316.	2.3	17
22	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
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	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
25	Electronic structure calculations of rare-earth intermetallic compound YAg using ab initio methods. Journal of Rare Earths, 2009, 27, 664-666.	2.5	13
26	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
27	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
28	Structural, elastic, electronic and thermoelectric properties of XPN₂ (X =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.0	11
29	First principles study of elastic and mechanical properties of TlBr and TlCl compounds. Journal of Molecular Structure, 2020, 1200, 127150.	1.8	11
30	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
31	Structural, electronic and elastic properties of YCu from first principles. Journal of Rare Earths, 2009, 27, 661-663.	2.5	10
32	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
33	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
34	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
35	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
36	Electronic and phonon structures of AuGa2and AuIn2. Journal of Physics Condensed Matter, 2006, 18, 6777-6784.	0.7	9

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37	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
38	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
39	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
40	Elastic, mechanical, anisotropic, optical and magnetic properties of V₂NiSb Heusler alloy. Physica Scripta, 2021, 96, 035807.	1.2	9
41	Three-body effect on the lattice dynamics of Pdâ€“10% Fe alloys. Physical Review B, 1995, 51, 3458-3461.	1.1	8
42	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
43	First principles study of the electronic, optical, elastic and thermoelectric properties of Nb2WNi alloy. Molecular Physics, 0, , e1928314.	0.8	8
44	Ab initiocalculation of the ground-state properties of CoSi2. Journal of Physics Condensed Matter, 2005, 17, 7127-7132.	0.7	7
45	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
46	Structural, elastic, electronic, phonon and thermal properties of Ir₃Ta and Rh₃Ta alloys. Philosophical Magazine Letters, 2015, 95, 392-400.	0.5	7
47	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
48	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
49	DFT aspects of the elastic, mechanical, magnetic, thermodynamic and optical properties of Ce3XY perovskites. Philosophical Magazine, 0, , 1-20.	0.7	7
50	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
51	STRUCTURAL, ELECTRONIC AND PHONON PROPERTIES OF LaX COMPOUNDS (X = P, As). International Journal of Modern Physics B, 2008, 22, 5027-5033.	1.0	6
52	Elastic and mechanical properties of Mg3Rh intermetallic compound: An ab initio study. Journal of Magnesium and Alloys, 2016, 4, 123-127.	5.5	6
53	Insight into the optoelectronic and thermoelectric properties of Ca-based Zintl phase CaCd 2 X 2 (X =) Tj ETQq1 1 0.784314 rgBT /Ov	1.3	6
54	Structural, elastic and mechanical properties of Tiâ€“15Nbâ€“xGe alloys: insight from DFT calculations. Bulletin of Materials Science, 2021, 44, 1.	0.8	6

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55	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
56	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
57	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
58	Optoelectronic and thermoelectric properties of Zintl YLi ₃ A ₂ () Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 107801.	0.7	5
59	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
60	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
61	Effect of Structure on the Electronic, Magnetic and Thermal Properties of Cubic Fe2MnxNi1â^'xSi Heusler Alloys. Journal of Electronic Materials, 2019, 48, 337-351.	1.0	5
62	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
63	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
64	Ground state and phonon spectrum of NiSi2. Philosophical Magazine, 2011, 91, 468-476.	0.7	4
65	First-principles study of B2-like intermetallics LaMg and YMg. Intermetallics, 2012, 22, 218-225.	1.8	4
66	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
67	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
68	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
69	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
70	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
71	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
72	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

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73	First principles study of the structural, elastic, electronic and phonon properties of CdX2O4 (X=Al,) Tj ETQq1 1 0.784314 rgBT /Overlo		3
74	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
75	Electronic structure and magnetic properties of manganese-based MnAs1â^'xPx ternary alloys. Journal of Magnetism and Magnetic Materials, 2019, 469, 329-341.	1.0	3
76	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
77	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
78	Prediction of the electronic structure, optical and vibrational properties of ScXCo2Sb2 (Xâ€‰=â€‰V, Nb and) Tj ETQq0 0 0 rgBT /Over	0.9	3
79	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
80	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
81	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
82	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
83	Electronic, mechanical, and optical properties of Ruddlesden-Popper perovskite sulfides: First principle calculation. Ferroelectrics, 2018, 535, 142-151.	0.3	2
84	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
85	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
86	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
87	Phonon Dispersion of Fe-30%Mn Alloy. Physica Scripta, 1999, 60, 569-571.	1.2	1
88	Vibrational properties of the Sb:InP() surface. Surface Science, 2002, 507-510, 1-6.	0.8	1
89	First-principles investigation of structural, electronic and dynamical properties in ScAuSn alloy. Computational Materials Science, 2007, 41, 134-137.	1.4	1
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	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
92	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
93	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
94	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
95	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
96	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
97	Elastic properties of antiferromagnetic Fe-40%Mn alloy. Journal of Materials Science Letters, 2000, 19, 127-129.	0.5	0
98	Structural, Electronic and Dynamical Properties of GeSi: An Ab-initio Study. AIP Conference Proceedings, 2007, , .	0.3	0
99	Ab-initio Study of Electronic Structure of ScAuSn. AIP Conference Proceedings, 2007, , .	0.3	0
100	First-Principle Calculations of Electronic and Dynamical Properties of GeSn. AIP Conference Proceedings, 2007, , .	0.3	0
101	Ab initio study of structural, electronic and dynamical properties of MgAuSn. European Physical Journal B, 2007, 58, 319-322.	0.6	0
102	Preface of the â€œSymposium on first-principles investigation of structural, electronic, elastic, thermodynamic and phonon properties of materialsâ€•, 2014, , .		0
103	Structural, elastic, electronic and phonon properties of SnX2O4 (X=Mg, Zn, Cd) spinel from density functional theory. AIP Conference Proceedings, 2014, , .	0.3	0
104	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
105	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
106	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
107	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
108	Investigation of Elastic Anisotropy Pressure Change in Al-Sc Alloys. El-Cezeri Journal of Science and Engineering, 0, , .	0.1	0

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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