Sule Ugur

List of Publications by Year in Descending Order

97 papers	713 citations	15 h-index	21 g-index
107 ext. papers	938 ext. citations	2.6 avg, IF	4.46 L-index

#	Paper	IF	Citations
97	Electronic, elastic, mechanical and anisotropic response of W3XC2 (X: Si, Ge and Al) alloys via first-principles. *Solid State Communications*, **2022**, 343, 114648	1.6	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	4.4	1
95	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	3.3	1
94	Exploring the elastic, mechanical and anisotropic response of Ti-5Al-XSn alloys through DFT calculations. *Chinese Journal of Physics*, **2022**, 77, 151-160	3.5	0
93	Dynamical and mechanical stability, electronic properties, bonding and weak interactions analysis of new compounds MgS2 and MgSe2 in Pa3? space group structure: Ab initio study. *Materials Science in Semiconductor Processing*, **2022**, 146, 106659	4.3	1
92	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**, 413851	2.8	0
91	A first-principles study for the elastic and mechanical properties of Ti64, Ti6242 and Ti6246 alloys. *European Physical Journal B*, **2021**, 94, 1	1.2	2
90	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	2.5	1
89	Elastic isotropy, magnetic and electronic properties, bonding and non-covalent interactions analyses of HoFe4P12 filled-skutterudite: DFT + U + SOC, QTAIM and NCI investigations. *Journal of Magnetism and Magnetic Materials*, **2021**, 518, 167435	2.8	3
88	Elastic, mechanical, optical and magnetic properties of Ru2MnX (X = Nb, Ta, V) Heusler alloys. *Journal of Magnetism and Magnetic Materials*, **2021**, 523, 167614	2.8	8
87	Electronic structure, optical and vibrational properties of Ti2FeNiSb2 and Ti2Ni2InSb double half heusler alloys. *Materials Science in Semiconductor Processing*, **2021**, 123, 105531	4.3	6
86	Elastic, mechanical, anisotropic, optical and magnetic properties of V2NiSb Heusler alloy. *Physica Scripta*, **2021**, 96, 035807	2.6	5
85	First principles study of electronic, elastic, optical and magnetic properties of Rh2MnX (X = Ti, Hf, Sc, Zr, Zn) Heusler alloys. *International Journal of Quantum Chemistry*, **2021**, 121, e26606	2.1	5
84	Structural, elastic and mechanical properties of Ti15NbxGe alloys: insight from DFT calculations. *Bulletin of Materials Science*, **2021**, 44, 1	1.7	3
83	First principles study of structural, elastic, mechanical and electronic properties of nitrogen-doped cubic diamond. *Bulletin of Materials Science*, **2021**, 44, 1	1.7	11
82	Study of structural, elastic, electronic, and vibrational properties of MRhO (M = Cd and Zn) spinels: DFT-based calculations. *Journal of Molecular Modeling*, **2020**, 26, 140	2	1
81	A theoretical study for the band gap energies of the most common silica polymorphs. *Chinese Journal of Physics*, **2020**, 65, 472-480	3.5	4

80	Pressure induced phase transition, electronic and optical properties of LiBeX (X = As, Sb and Bi). *Journal of Physics Condensed Matter*, **2020**, 32, 325503	1.8	2
79	Cation distribution effect on electronic, magnetic structure and optic properties in cobalt ferrites (Co 1− y Fe y) Tet (Co y Fe 2− y) Oct O 4 with disordered spinel structure. *Physica Scripta*, **2020**, 95, 105801	2.6	2
78	DFT-investigation on anisotropy degree of electronic, optical, and mechanical properties of olivine ZnRE2S4 (RE = Er, Tm) compounds. *Materials Research Express*, **2020**, 7, 016305	1.7	2
77	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	2.8	6
76	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	1.5	4
75	First principles investigations of structural, elastic, mechanical, electronic and optical properties of triple perovskite Ba2K2Te2O9. *Physica B: Condensed Matter*, **2020**, 596, 412404	2.8	8
74	An ab-initio investigation of the electronic structure, chemical bonding and optical properties of Ba2HgS5 semiconductor. *Molecular Physics*, **2020**, 118, e1587026	1.7	4
73	First principles study of elastic and mechanical properties of TlBr and TlCl compounds. *Journal of Molecular Structure*, **2020**, 1200, 127150	3.4	8
72	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	2.8	12
71	Structural, elastic, electronic and thermoelectric properties of XPN2 (X = Li, Na): First-principles study. *International Journal of Modern Physics B*, **2019**, 33, 1950234	1.1	2
70	First Brillouin zone-centre phonon frequencies and elastic stiffness of the Ln2Hf2O7 (Ln= La, Nd, Sm and Eu) pyrochlore. *Computational Condensed Matter*, **2019**, 21, e00428	1.7	0
69	Lattice dynamical and elastic properties of BaFX (X = Cl, Br and I): Matlockite structure compounds. *International Journal of Modern Physics B*, **2019**, 33, 1950221	1.1	2
68	Structural, electronic, optical and elastic properties of XLa2S4 (X = Ba; Ca): Ab initio study. *Physica B: Condensed Matter*, **2019**, 558, 91-99	2.8	5
67	Insight into the structural, elastic, electronic, thermoelectric, thermodynamic and optical properties of MRhSb (M = Ti, Zr, Hf) half-Heuslers from ab initio calculations. *Chinese Journal of Physics*, **2019**, 59, 434-448	3.5	8
66	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	1.7	2
65	Structural, elastic, electronic and vibrational properties of XAl2O4 (X = Ca, Sr and Cd) semiconductors with orthorhombic structure. *Journal of Alloys and Compounds*, **2019**, 809, 151773	5.7	6
64	Phase transitions and lattice dynamics in perovskite-type hydride [Formula: see text]. *Journal of Physics Condensed Matter*, **2019**, 31, 505402	1.8	0
63	Pressure effect on mechanical stability and ground state optoelectronic properties of Li2S2 produced by Lithium–Sulfur batteries discharge: GGA-PBE, GLLB-SC and mBJ investigation. *Philosophical Magazine*, **2019**, 99, 2789-2817	1.6	1

62	First principles investigations of the structural, elastic, vibrational, and thermodynamic properties of TiMgO oxide spinels: cubic and tetragonal phases. *Journal of Molecular Modeling*, **2019**, 25, 210	2	0
61	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	
60	Theoretical research on structural, electronic, mechanical, lattice dynamical and thermodynamic properties of layered ternary nitrides Ti2AN (A = Si, Ge and Sn). *Journal of Alloys and Compounds*, **2019**, 771, 664-673	5.7	18
59	Electronic structure and magnetic properties of manganese-based MnAs1−xPx ternary alloys. *Journal of Magnetism and Magnetic Materials*, **2019**, 469, 329-341	2.8	2
58	Effect of Structure on the Electronic, Magnetic and Thermal Properties of Cubic Fe2MnxNi1−xSi Heusler Alloys. *Journal of Electronic Materials*, **2019**, 48, 337-351	1.9	3
57	First-principle calculations of structural, electronic and magnetic investigations of Mn2RuGe1-xSnx quaternary Heusler alloys. *Chinese Journal of Physics*, **2018**, 56, 567-573	3.5	54
56	Structural, electronic, elastic, optical and vibrational properties of MAl2O4 (M = Co and Mn) aluminate spinels. *Ceramics International*, **2018**, 44, 310-316	5.1	13
55	External pressure effect on the electronic, optical and thermoelectric properties of the CdY2Ch4 (Ch = S, Se) spinel compounds: Via modified Becke−Johnson (mBJ) exchange potential. *Physica B: Condensed Matter*, **2018**, 545, 40-47	2.8	6
54	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	5.7	20
53	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	2.8	4
52	Ab-Initio Calculations and Thermodynamic Description of the Yb-Cd and Yb-Sn Systems. *Journal of Phase Equilibria and Diffusion*, **2017**, 38, 665-675	1	
51	Investigation of the structural, electronic, elastic and thermodynamic properties of Curium Monopnictides: An ab−initio study. *International Journal of Modern Physics B*, **2017**, 31, 1750226	1.1	4
50	Electron-phonon superconductivity in the ternary phosphides BaM2P2 (M=Ni,Rh,and Ir). *Physical Review B*, **2016**, 94,	3.3	9
49	Theoretical investigation of superconductivity in SrPd2Ge2, SrPd2As2, and CaPd2As2. *Physical Review B*, **2016**, 93,	3.3	4
48	Investigation of electronic structure and thermodynamic properties of quaternary Li-containing chalcogenide diamond-like semiconductors. *Semiconductor Science and Technology*, **2016**, 31, 125015	1.8	1
47	Structural, electronic, optical and elastic properties of the complex K2PtCl6-structure hydrides ARuH6 (A = Mg, Ca, Sr and Ba): first-principles study. *Philosophical Magazine*, **2016**, 96, 2328-2361	1.6	14
46	Electronic structure, optical and thermodynamic properties of ternary hydrides MBeH3 (M = Li, Na, and K). *Canadian Journal of Physics*, **2016**, 94, 865-876	1.1	3
45	First principles study of hydrogen storage material NaBH4and LiAlH4compounds: electronic structure and optical properties. *Physica Scripta*, **2016**, 91, 045804	2.6	13

44	First-principles investigation of superconductivity in the body-centred tetragonal. *Philosophical Magazine*, **2016**, 96, 2059-2073	1.6	5
43	Optoelectronic and thermoelectric properties of Zintl YLi 3 A 2 (A = Sb, Bi) compounds through modified Becke□ohnson potential. *Chinese Physics B*, **2016**, 25, 107801	1.2	2
42	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	3.9	10
41	Structural, elastic, electronic, phonon and thermal properties of Ir3Ta and Rh3Ta alloys. *Philosophical Magazine Letters*, **2015**, 95, 392-400	1	3
40	Thermodynamic description of the Bi□s and Bi□m system supported by first-principles calculations. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2015**, 48, 72-78	1.9	9
39	Structural phase transition and opto-electronic properties of NaZnAs. *Journal of Alloys and Compounds*, **2015**, 622, 812-818	5.7	1
38	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	3.9	17
37	Ab initio investigation of BCS-type superconductivity in LuNi2B2C-type superconductors. *Physical Review B*, **2015**, 92,	3.3	30
36	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	1.6	3
35	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	0.3	
34	Electronic and phonon properties of the full-Heusler alloys X2YAl (X = Co, Fe and Y = Cr, Sc): a density functional theory study. *Journal of Materials Science*, **2014**, 49, 4180-4190	4.3	34
33	Phase transition of Nowotny□uza 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	3.2	16
32	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	2.4	6
31	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	3.2	22
30	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	1.1	11
29	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	1	22
28	Elastic and thermodynamic properties of ZnSc2S4 and CdSc2S4 compounds under pressure and temperature effects. *Computational Materials Science*, **2013**, 70, 107-113	3.2	18
27	Structural, elastic, electronic and phonon properties of scandium-based compounds ScX3 (X=Ir, Pd, Pt and Rh): An ab initio study. *Computational Materials Science*, **2013**, 79, 703-709	3.2	19

26	Prediction Study of the Mechanical and Thermodynamic Properties of the (hbox {RBRh}_{3}) (R (=) Sm, Eu, Gd, and Tb) Compounds. *International Journal of Thermophysics*, **2013**, 34, 2102-2118	2.1	
25	A first-principles study of the structural, elastic, electronic and phonon properties of LiMgP and LiMgAs in the and phases. *Journal of Alloys and Compounds*, **2013**, 551, 108-117	5.7	4
24	Structural, electronic and vibrational properties of ordered intermetallic alloys CoZ (Z = Al, Be, Sc and Zr) from first-principles total-energy calculations. *Philosophical Magazine*, **2013**, 93, 3260-3277	1.6	9
23	Structural, Elastic, Electronic and Optical Properties of Cu3TMSe4 (TM = V, Nb and Ta) Sulvanite Compounds via First-Principles Calculations. *Science of Advanced Materials*, **2013**, 5, 97-106	2.3	24
22	AB INITIO STUDY OF PHONON DISPERSION AND ELASTIC PROPERTIES OF L12 INTERMETALLICS Ti3Al AND Y3Al. *Modern Physics Letters B*, **2013**, 27, 1350224	1.6	2
21	First-principles study of B2-like intermetallics LaMg and YMg. *Intermetallics*, **2012**, 22, 218-225	3.5	2
20	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	3.2	4
19	Ab initio study of some fundamental physical properties of the cubic inverse-perovskite Mn3ZnC and Mn3GeC. *Computational Materials Science*, **2012**, 58, 162-166	3.2	3
18	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	1.1	9
17	Full-Potential Calculation of Structural, Electronic, and Thermodynamic Properties of Fluoroperovskite (text{ CsMF}_{3}) (M = Be and Mg). *International Journal of Thermophysics*, **2012**, 33, 2339-2350	2.1	2
16	Electronic and phonon properties of Sc-TM (TM=Ag, Cu, Pd, Rh, Ru) compounds. *Computational Materials Science*, **2010**, 47, 668-671	3.2	14
15	Phonon and elastic properties of AlSc and MgSc from first-principles calculations. *Computational Materials Science*, **2010**, 48, 866-870	3.2	23
14	Structural, electronic and phonon properties of MoTa and MoNb: a density functional investigation. *Physica Scripta*, **2010**, 82, 015601	2.6	1
13	Theoretical study of the phonon properties of SrS. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2009**, 162, 116-119	3.1	18
12	Structural, electronic and elastic properties of YCu from first principles. *Journal of Rare Earths*, **2009**, 27, 661-663	3.7	8
11	Electronic structure calculations of rare-earth intermetallic compound YAg using ab initio methods. *Journal of Rare Earths*, **2009**, 27, 664-666	3.7	12
10	STRUCTURAL, ELECTRONIC AND PHONON PROPERTIES OF LaX COMPOUNDS (X = P, As). *International Journal of Modern Physics B*, **2008**, 22, 5027-5033	1.1	4
9	Structural, electronic and phonon properties investigation of YP and YAs compounds. *Journal of Physics and Chemistry of Solids*, **2008**, 69, 791-798	3.9	20

8	First principles linear response calculations of phonons for ScP and ScAs. *Solid State Communications*, **2008**, 147, 198-200	1.6	11
7	First-principles investigation of structural, electronic and dynamical properties in ScAuSn alloy. *Computational Materials Science*, **2007**, 41, 134-137	3.2	0
6	Energy/power breakdown of pipelined nanometer caches (90nm/65nm/45nm/32nm) **2006**,		14
5	First-principles study of surface phonons on the AlN(110) surface. *Surface Science*, **2004**, 566-568, 904-908	1.88	2
4	Phonon Dispersion of Fe-30%Mn Alloy. *Physica Scripta*, **1999**, 60, 569-571	2.6	0
3	Investigating the Magnetic, Mechanical, Electronic, Optical, and Anisotropic Properties of ZrCoFeX (X = Si, Ge) Quaternary Heusler Alloys via First Principles. *Journal of Superconductivity and Novel Magnetism*,1	1.5	
2	DFT aspects of the elastic, mechanical, magnetic, thermodynamic and optical properties of Ce3XY perovskites. *Philosophical Magazine*,1-20	1.6	0
1	First principles study of the electronic, optical, elastic and thermoelectric properties of Nb2WNi alloy. *Molecular Physics*,e1928314	1.7	3