Gkay Ugur

List of Publications by Year in Descending Order

98 papers	701 citations	13 h-index	21 g-index
111 ext. papers	909 ext. citations	2.6 avg, IF	4.34 L-index

#	Paper	IF	Citations
98	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
97	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
96	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
95	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
94	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
93	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
92	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
91	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
90	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
89	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
88	Elastic, mechanical, anisotropic, optical and magnetic properties of V2NiSb Heusler alloy. *Physica Scripta*, **2021**, 96, 035807	2.6	5
87	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
86	Structural, elastic and mechanical properties of Ti5NbGe alloys: insight from DFT calculations. *Bulletin of Materials Science*, **2021**, 44, 1	1.7	3
85	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
84	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
83	Cation distribution effect on electronic, magnetic structure and optic properties in cobalt ferrites (Co 1 Fe y) Tet (Co y Fe 2) Oct O 4 with disordered spinel structure. *Physica Scripta*, **2020**, 95, 105801	2.6	2
82	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

81	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
80	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
79	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
78	First principles study of elastic and mechanical properties of TlBr and TlCl compounds. *Journal of Molecular Structure*, **2020**, 1200, 127150	3.4	8
77	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
76	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
75	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
74	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
73	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
72	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
71	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	1	2
70	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
69	Phase transitions and lattice dynamics in perovskite-type hydride [Formula: see text]. *Journal of Physics Condensed Matter*, **2019**, 31, 505402	1.8	0
68	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
67	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
66	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	
65	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
64	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

63	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
62	Insight into the optoelectronic and thermoelectric properties of Ca-based Zintl phase CaCd 2 X 2 (X = P, As) from first principles calculation. *Physica B: Condensed Matter*, **2018**, 538, 35-46	2.8	4
61	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
60	The effect of martensitic phase transition from cubic to tetragonal on the physical properties of V3Si superconductor. *Intermetallics*, **2018**, 96, 25-32	3.5	2
59	Structural, electronic, elastic, optical and vibrational properties of MAl2O4 (M = Co and Mn) aluminate spinels. *Ceramics International*, **2018**, 44, 310-316	5.1	13
58	External pressure effect on the electronic, optical and thermoelectric properties of the CdY2Ch4 (Ch = S, Se) spinel compounds: Via modified Becke−ohnson (mBJ) exchange potential. *Physica B: Condensed Matter*, **2018**, 545, 40-47	2.8	6
57	Electronic, mechanical, and optical properties of Ruddlesden-Popper perovskite sulfides: First principle calculation. *Ferroelectrics*, **2018**, 535, 142-151	0.6	2
56	Band Structure and Optical Properties of Kesterite Type Compounds: first principle calculations. *IOP Conference Series: Materials Science and Engineering*, **2017**, 175, 012014	0.4	0
55	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
54	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
53	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	
52	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
51	Computational investigations on band structure and electronic features of chromium-based carbides and nitride Cr3PX (X=C and N) through the FP-APW+LO approach. *Superlattices and Microstructures*, **2017**, 109, 1-12	2.8	5
50	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
49	Elastic and mechanical properties of Mg3Rh intermetallic compound: An ab initio study. *Journal of Magnesium and Alloys*, **2016**, 4, 123-127	8.8	6
48	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
47	First principles study of hydrogen storage material NaBH4and LiAlH4compounds: electronic structure and optical properties. *Physica Scripta*, **2016**, 91, 045804	2.6	13
46	First-principles study of structural, electronic, elastic and phonon properties of AB2O4(A = Ge,Si;B = Mg,Zn,Cd) spinel oxides. *Modern Physics Letters B*, **2016**, 30, 1650002	1.6	7

45	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
44	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
43	Structural, elastic, electronic, phonon and thermal properties of Ir3Ta and Rh3Ta alloys. *Philosophical Magazine Letters*, **2015**, 95, 392-400	1	3
42	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
41	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
40	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	
39	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
38	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
37	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
36	First principles study of the structural, elastic, electronic and phonon properties of CdX2O4 (X=Al, Ga, In) spinel-type oxides **2014**,		1
35	Elastic and thermodynamic properties of ZnSc2S4 and CdSc2S4 compounds under pressure and temperature effects. *Computational Materials Science*, **2013**, 70, 107-113	3.2	18
34	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
33	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
32	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	5.7	71
31	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
30	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
29	First-principles study of B2-like intermetallics LaMg and YMg. *Intermetallics*, **2012**, 22, 218-225	3.5	2
28	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

27	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
26	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
25	Ground state and phonon spectrum of NiSi2. *Philosophical Magazine*, **2011**, 91, 468-476	1.6	3
24	Phonon and elastic properties of AlSc and MgSc from first-principles calculations. *Computational Materials Science*, **2010**, 48, 866-870	3.2	23
23	Structural, electronic and phonon properties of MoTa and MoNb: a density functional investigation. *Physica Scripta*, **2010**, 82, 015601	2.6	1
22	Structural, electronic and elastic properties of YCu from first principles. *Journal of Rare Earths*, **2009**, 27, 661-663	3.7	8
21	Electronic structure calculations of rare-earth intermetallic compound YAg using ab initio methods. *Journal of Rare Earths*, **2009**, 27, 664-666	3.7	12
20	STRUCTURAL, ELECTRONIC AND PHONON PROPERTIES OF LaX COMPOUNDS (X = P, As). *International Journal of Modern Physics B*, **2008**, 22, 5027-5033	1.1	4
19	Ab initio study of structural, electronic and dynamical properties of MgAuSn. *European Physical Journal B*, **2007**, 58, 319-322	1.2	
18	First-principles investigation of structural, electronic and dynamical properties in ScAuSn alloy. *Computational Materials Science*, **2007**, 41, 134-137	3.2	0
17	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	3.5	5
16	Electronic and phonon structures of AuGa2and AuIn2. *Journal of Physics Condensed Matter*, **2006**, 18, 6777-6784	1.8	9
15	Theoretical study of the structural, electronic and dynamical properties of rocksalt ScN and GaN. *Diamond and Related Materials*, **2006**, 15, 1175-1178	3.5	20
14	Structural and dynamical properties of zinc-blende GaN, AlN, BN, and their (110) surfaces. *Physical Review B*, **2005**, 71,	3.3	46
13	Ab initiocalculation of the ground-state properties of CoSi2. *Journal of Physics Condensed Matter*, **2005**, 17, 7127-7132	1.8	7
12	First-principles study of electronic and dynamical properties of AuAl2. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2004**, 1, 3027-3030		10
11	Vibrational properties of the Sb:InP(110) surface. *Surface Science*, **2002**, 507-510, 1-6	1.8	1
10	Elastic properties of antiferromagnetic Fe-40%Mn alloy. *Journal of Materials Science Letters*, **2000**, 19, 127-129		

9	Phonon Dispersion of Fe-30%Mn Alloy. *Physica Scripta*, **1999**, 60, 569-571	2.6	0
8	The Lattice Dynamics of Ni-24%Fe Alloy Based on an Empirical Many-Body Potential. *Acta Physica Polonica A*, **1999**, 96, 391-398	0.6	
7	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		2
6	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		2
5	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		2
4	Three-body effect on the lattice dynamics of Pd-10% Fe alloys. *Physical Review B*, **1995**, 51, 3458-3461	3.3	8
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