

# Prof. GÖKAY UĞUR

## Personal Information

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## International Researcher IDs

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Publons / Web Of Science ResearcherID: B-6223-2016

ScopusID: 55908046100

Yoksis Researcher ID: 109510

## Education Information

Doctorate, Gazi University, Fen Bilimleri Enstitüsü, Fizik (Dr), Turkey 1995 - 1999

Postgraduate, Gazi University, Fen Bilimleri Enstitüsü, Fizik (YI) (Tezli), Turkey 1990 - 1994

Undergraduate, Ankara University, Mühendislik Fakültesi, Fizik Mühendisliği Bölümü, Turkey 1985 - 1988

## Dissertations

Doctorate, Bazı Fe-bazlı alaşımların örgü dinamiği ve bir ince film çalışması, Gazi University, Fen Bilimleri Enstitüsü, Fizik (Dr), 1999

Postgraduate, Fe1-xPdx (X=0,28 0,90 0,96) alaşımlarında örgü dinamiği, Gazi University, Fen Bilimleri Enstitüsü, Fizik (YI) (Tezli), 1994

## Research Areas

Physics, Condensed Matter 1: Structural, Mechanical and Thermal Properties, Intensive Article 2: Electronic Structure, Electric, Magnetic and Optical Properties

## Academic Titles / Tasks

Professor, Gazi University, Fen Fakültesi, Fizik, 2013 - Continues

Associate Professor, Gazi University, Fen Fakültesi, Fizik, 2008 - 2013

Assistant Professor, Gazi University, Fen Fakültesi, Fizik, 2002 - 2008

Research Assistant, Gazi University, Fen Fakültesi, Fizik, 1993 - 2002

## Academic and Administrative Experience

Bölüm Akademik Teşvik Değerlendirme Komisyonu Üyesi, Gazi University, Fen Fakültesi, Fizik, 2019 - 2020

Fakülte Yönetim Kurulu Üyesi, Gazi University, Polatlı Fen-Edebiyat Fakültesi, Fizik, 2017 - 2020

BAP Scientific Commissioner, Gazi University, Rektörlük, Gazi Üniversitesi, 2016 - 2020

Head of Department, Gazi University, Fen Fakültesi, Fizik, 2014 - 2017

BAP Scientific Commissioner, Gazi University, Fen Fakültesi, Fizik, 2013 - 2016  
Gazi University, Fen Fakültesi, Fizik Bölümü, 2007 - 2008

## Courses

83FBE5002 YÜKSEK LİSANS TEZ ÇALIŞMASI, Postgraduate, 2023 - 2024  
83FBE6002 DOKTORA TEZ ÇALIŞMASI, Doctorate, 2023 - 2024  
FİZ255 FİZİK LABORATUVARI (MATEMATİK BÖLÜMÜ), Undergraduate, 2023 - 2024  
FİZ103 FİZİK I (TEKNOLOJİ FAKÜLTESİ), Undergraduate, 2023 - 2024  
FİZ251 FİZİK LABORATUVARI II (ELEKTRİK), Undergraduate, 2023 - 2024

## Advising Theses

Uğur G., Theoretical investigation of the structural, electronic, elastic, phonon and optical properties of  $X_2MgS_4$  ( $X=Sc, Y, Cd$ ) compounds in cubic structure, Postgraduate, E.TOK(Student), 2023  
UĞUR G., Optical Design Of The Lens Group For Visible And Infrared Applications, Postgraduate, A.EREN(Student), 2020  
UĞUR G., Theoretical Investigation Of The Structural, Electronic, Elastic, Vibrational And Thermodynamic Properties Of Some Ternary Compounds In Cubic Spinel Structure, Doctorate, A.CANDAN(Student), 2016  
UĞUR G., Investigation of the ground state properties of TlBr and TlCl compounds using density functional theory, Postgraduate, Ö.KÖKER(Student), 2014  
UĞUR G., Radyasyon tedavisinde kullanılan 6 MV foton enerjisinin tümörlü dokuya uygulama süresini hesaplayan bilgisayar programının yazılması, Postgraduate, Y.ERGİN(Student), 2014  
UĞUR G., The investigation of the electronic, elastic and vibrational properties of cubic  $Fe_2YSi$  ( $Y=Co, Cr, Mn$  and  $Ni$ ) heusler compounds within the density functional theory, Postgraduate, F.EKİNCİ(Student), 2011  
UĞUR G., The investigation of the structural, electronic, elastic and vibrational properties NaCl and CsCl structures zirconium carbide ve zirconium nitride compounds with the density functional theory, Postgraduate, A.KARADUMAN(Student), 2011  
UĞUR G., Investigation of  $Co_2MnX$  ( $X=Al, Ga, Ge, Si$ ) heusler alloys, in cubic form, in terms of their structural, electronic, elastic and vibrational properties using density functional theory, Postgraduate, A.CANDAN(Student), 2011  
UĞUR G., THE INVESTIGATION OF THE ELECTRONIC AND VIBRATIONAL PROPERTIES OF SOME COMPOUNDS WITHIN THE DENSITY FUNCTIONAL THEORY, Postgraduate, A.ERKİŞİ(Student), 2007  
UĞUR G., Bazı kristallerin elastik ve titreşim özelliklerinin varshni potansiyel fonksiyonu ile incelenmesi, Postgraduate, M.DİNÇER(Student), 2007  
UĞUR G.,  $MgAuSn$  bileşiğinin elektronik yapısının ve titreşim özelliklerinin yoğunluk fonksiyon teorisi ile incelenmesi, Doctorate, N.ARIKAN(Student), 2006  
UĞUR G., Yoğunluk fonksiyon teorisi ile bazı bileşiklerin elektronik yapılarının ve titreşim özelliklerinin teorik olarak incelenmesi, Doctorate, F.SOYALP(Student), 2006  
UĞUR G., Si(111)- (7x7) yüzeyinin değişik sıcaklıklarda STM ile incelenmesi, Postgraduate, C.ALAŞALVAR(Student), 2006  
UĞUR G., Si üzerine büyütülmüş Au (111) yüzeyinin taramalı tünelleme mikroskop ile incelenmesi, Postgraduate, U.NİYZAZI(Student), 2006  
UĞUR G.,  $AuAl_2$  bileşiğinin elektronik yapısının ve titreşim özelliklerinin yoğunluk fonksiyon teorisi ile incelenmesi, Postgraduate, H.ALTUNTAŞ(Student), 2004

## Published journal articles indexed by SCI, SSCI, and AHCI

1. **A comprehensive theoretical investigation of the structural, elastic, electronic, optical, thermal, and catalytic properties of the monoclinic perovskite  $ScRhO_3$**   
Foudia L., Reffas M., Haddadi K., Hamici M., Messalti A. S., UĞUR G.

MATERIALS SCIENCE IN SEMICONDUCTOR PROCESSING, vol.185, 2025 (SCI-Expanded)

- II. **Impact of Ir doping on the thermoelectric transport properties of half-Heusler alloys**  
Abdelkebir B., Semari F., Charifi Z., Baaziz H., Ghellab T., UĞUR Ş., UĞUR G., Khenata R.  
PHYSICA SCRIPTA, vol.99, no.11, 2024 (SCI-Expanded)
- III. **Structural, electronic, elastic and optical properties of double spinel  $MgAlGaO_4$ : a DFT investigation**  
Kushwaha A., GÜLER E., ÖZDEMİR A., GENÇ A. E., UĞUR G.  
INDIAN JOURNAL OF PHYSICS, vol.98, no.12, pp.4011-4017, 2024 (SCI-Expanded)
- IV. **Investigation on the hydrogen storage properties, electronic, elastic, and thermodynamic of Zintl Phase Hydrides  $XGaSiH$  ( $X = sr, ca, ba$ )**  
Ammi H., Charifi Z., Baaziz H., Ghellab T., Bouhdjer L., Adalla S., Ocak H. Y., UĞUR Ş., UĞUR G.  
INTERNATIONAL JOURNAL OF HYDROGEN ENERGY, vol.87, pp.966-984, 2024 (SCI-Expanded)
- V. **Theoretical Predictions for Elastic, Mechanical, Anisotropic, Electronic, and Optical Profiles of Wurtzite CdS, CdSe, and CdTe**  
Guler E., UĞUR Ş., Guler M., UĞUR G.  
JOM, 2024 (SCI-Expanded)
- VI. **First principles investigations of the electronic, elastic, mechanical, anisotropic, optical, and thermoelectric performance of monoclinic SiGe semiconductors**  
GÜLER E., GÜLER M., UĞUR Ş., UĞUR G.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS B, no.26, 2024 (SCI-Expanded)
- VII. **DFT analysis of the electronic, optical, phonon, elastic, and mechanical features of ternary  $Rb_2XS_3$  ( $X = Si, Ge, Sn$ ) chalcogenides**  
UĞUR Ş., GÜLER M., ÖZDEMİR A., GÜLER E., UĞUR G.  
OPTICAL AND QUANTUM ELECTRONICS, vol.56, no.7, 2024 (SCI-Expanded)
- VIII. **Molecular dynamics exploration of the temperature-dependent elastic, mechanical, and anisotropic properties of hcp ruthenium**  
GÜLER E., UĞUR Ş., GÜLER M., UĞUR G.  
EUROPEAN PHYSICAL JOURNAL PLUS, vol.139, no.5, 2024 (SCI-Expanded)
- IX. **Structural and mechanical investigation of a  $TiAl_2$  based alloy: A combined theoretical and experimental study**  
Mermer E., Çinici H., Uğur G., Ünal R.  
MATERIALS LETTERS, vol.354, 2024 (SCI-Expanded)
- X. **DFT predictions of the electronic, phonon, optical, and thermoelectric characteristics of  $CaCu_2S_2$**   
GÜLER E., GÜLER M., ÖZDEMİR A., GENÇ A. E., UĞUR G., UĞUR Ş.  
MRS COMMUNICATIONS, vol.13, no.6, pp.1320-1325, 2023 (SCI-Expanded)
- XI. **Unveiling the electronic, optical, and thermoelectrical properties of bulk and monolayer  $AlSiTe_3$  by first principles**  
GÜLER E., UĞUR Ş., GÜLER M., UĞUR G.  
CHEMICAL PHYSICS, vol.575, 2023 (SCI-Expanded)
- XII. **Development of an Al rich Ti-Al alloy with better ductility**  
Mermer E., Çinici H., Uğur G., Ünal R.  
VACUUM, vol.214, 2023 (SCI-Expanded)
- XIII. **Proposal of new stable Ru-based intermetallics,  $XRu_3$  ( $X = V, Nb$  and  $Ta$ ): Prediction of their bulk properties and their surfaces adsorption behavior and sensing properties to small gases**  
Saoudi A., Haddadi K., Medkour Y., Mosbah A., Reffas M., UĞUR G., Boukelkoul M., Bouriachi S.  
Vacuum, vol.213, 2023 (SCI-Expanded)
- XIV. **Investigating the electronic, elastic, mechanical, anisotropic, and optical aspects of  $Sc_2RuZ$  ( $Z: Al, Ga, and In$ ) full Heusler alloys from the first principles**  
GÜLER M., UĞUR Ş., GÜLER E., ÖZDEMİR A., Kushwaha A., GENÇ A. E., UĞUR G.  
PHYSICA B-CONDENSED MATTER, vol.659, 2023 (SCI-Expanded)

- XV. **A theoretical benchmark for the electronic, optical, and thermoelectrical characteristics of bulk and monolayer BiS<sub>2</sub>**  
 GÜLER E., UĞUR Ş., GÜLER M., UĞUR G.  
 MICRO AND NANOSTRUCTURES, vol.178, 2023 (SCI-Expanded)
- XVI. **Full potential theoretical investigations for electronic, optical, mechanical, elastic and anisotropic properties of X<sub>2</sub>Se<sub>2</sub>C (X = Ta, Nb) compounds**  
 Baaziz H., Ghellab T., Charifi Z., GÜLER M., UĞUR Ş., GÜLER E., GENÇ A. E., UĞUR G.  
 European Physical Journal B, vol.96, no.5, 2023 (SCI-Expanded)
- XVII. **Properties of the double half-Heusler alloy ScNbNi<sub>2</sub>Sn<sub>2</sub> with respect to structural, electronic, optical, and thermoelectric aspects**  
 Mekki H., Baaziz H., Charifi Z., Ghellab T., GENÇ A. E., UĞUR Ş., UĞUR G.  
 Solid State Communications, vol.363, 2023 (SCI-Expanded)
- XVIII. **Experimental investigations of the structural, morphologic and mechanical properties of Ti-18 %Nb-1.4 %Ge alloy**  
 Uğur G., Uğur Ş., Güler M., Güler E.  
 MATERIALS LETTERS, vol.335, 2023 (SCI-Expanded)
- XIX. **Revealing the electronic, optical, elastic, mechanical, anisotropic, and thermoelectric responses of Sc(2)NiZ (Z = Si, Ge, and Sn) Heusler alloys via DFT calculations**  
 GÜLER M., UĞUR Ş., UĞUR G., GÜLER E.  
 INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, vol.123, 2023 (SCI-Expanded)
- XX. **Prediction of the electronic structure, optical and vibrational properties of ScXCo<sub>2</sub>Sb<sub>2</sub> (X = V, Nb and Ta) double half-Heusler alloys: a theoretical study**  
 Charifi Z., Baaziz H., UĞUR Ş., UĞUR G.  
 INDIAN JOURNAL OF PHYSICS, vol.97, no.2, pp.413-428, 2023 (SCI-Expanded)
- XXI. **DFT exploration of the electronic, optical, phonon and thermoelectrical performances of bulk and monolayered AuCN**  
 UĞUR G., Güler M., UĞUR Ş., GÜLER E.  
 THEORETICAL CHEMISTRY ACCOUNTS, vol.142, no.2, 2023 (SCI-Expanded)
- XXII. **An ab initio study on phase stability, elastic and mechanical properties of Zr-doped TiAl<sub>2</sub> and α-TiAl<sub>3</sub> intermetallics**  
 Mermer E., ÇİNİCİ H., UĞUR G., ÜNAL R.  
 EPL, vol.140, no.3, 2022 (SCI-Expanded)
- XXIII. **Revealing the electronic, optical, phonon and thermoelectrical characteristics of bulk and monolayered RbLiS and RbLiSe compounds by DFT**  
 GÜLER E., UĞUR Ş., Güler M., ÖZDEMİR A., UĞUR G.  
 JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS, vol.170, 2022 (SCI-Expanded)
- XXIV. **Analyzing the electronic and optical properties of bulk, unstrained, and strained monolayers of SrS<sub>2</sub> by DFT**  
 Uğur Ş., Güler E., Güler M., Özdemir A., Uğur G.  
 PHYSICA E: LOW-DIMENSIONAL SYSTEMS AND NANOSTRUCTURES, vol.143, pp.115403, 2022 (SCI-Expanded)
- XXV. **Dynamical and mechanical stability, electronic properties, bonding and weak interactions analysis of new compounds MgS<sub>2</sub> and MgSe<sub>2</sub> in Pa( $\bar{3}$ ) space group structure: Ab initio study**  
 Bouafia H., UĞUR G., GÜLER M., GÜLER E., UĞUR Ş.  
 MATERIALS SCIENCE IN SEMICONDUCTOR PROCESSING, vol.146, 2022 (SCI-Expanded)
- XXVI. **The elastic, mechanical, and thermodynamic properties of NaXH<sub>4</sub> (X = B, Al) intended for the storage of hydrogen: An ab-initio study**  
 Ghellab T., Charifi Z., Baaziz H., Latteli H., Güler M., UĞUR Ş., GÜLER E., UĞUR G.  
 Physica B: Condensed Matter, vol.638, 2022 (SCI-Expanded)
- XXVII. **Exploring the elastic, mechanical and anisotropic response of Ti-5Al-XSn alloys through DFT**

calculations

Guler E., UĞUR Ş., Guler M., UĞUR G.

CHINESE JOURNAL OF PHYSICS, vol.77, pp.151-160, 2022 (SCI-Expanded)

- XXVIII. **Investigating the Magnetic, Mechanical, Electronic, Optical, and Anisotropic Properties of ZrCoFeX (X = Si, Ge) Quaternary Heusler Alloys via First Principles**  
Baaziz H., Ghellab T., Guler E., Charifi Z., UĞUR Ş., Guler M., UĞUR G.  
JOURNAL OF SUPERCONDUCTIVITY AND NOVEL MAGNETISM, vol.35, no.5, pp.1173-1182, 2022 (SCI-Expanded)
- XXIX. **First-principles calculations of electronic and optical properties of AgGa<sub>1-x</sub>TlxS<sub>2</sub> alloys: Analyses and design for solar cell applications**  
Mouacher R., Seddik T., Rezini B., Ul Haq B., Batouche M., Ugur G., UĞUR Ş., Belfedal A.  
JOURNAL OF SOLID STATE CHEMISTRY, vol.309, 2022 (SCI-Expanded)
- XXX. **Structural, elastic and mechanical properties of Hf-doped TiAl<sub>2</sub> and alpha-TiAl<sub>3</sub> intermetallic compounds: first-principle calculations**  
Mermer E., ÇİNİCİ H., UĞUR G., ÜNAL R.  
EUROPEAN PHYSICAL JOURNAL B, vol.95, no.5, 2022 (SCI-Expanded)
- XXXI. **Electronic, elastic, mechanical and anisotropic response of W<sub>3</sub>X<sub>2</sub> (X: Si, Ge and Al) alloys via first-principles**  
Güler E., Güler M., Uğur Ş., Özdemir A., Uğur G.  
SOLID STATE COMMUNICATIONS, vol.343, 2022 (SCI-Expanded)
- XXXII. **Chemical bonding, magnetic and electronic properties, mechanical and dynamical stabilities of DyOs<sub>4</sub>P<sub>12</sub> filled-skutterudite: DFT and QTAIM insight**  
Nekous M., Sahli B., Belarbi M., Bouafia H., Dorbane A., UĞUR Ş., UĞUR G.  
MATERIALS CHEMISTRY AND PHYSICS, vol.278, 2022 (SCI-Expanded)
- XXXIII. **DFT aspects of the elastic, mechanical, magnetic, thermodynamic and optical properties of Ce<sub>3</sub>XY perovskites**  
Guler E., Guler M., UĞUR Ş., Ugur G.  
PHILOSOPHICAL MAGAZINE, vol.102, no.3, pp.244-263, 2022 (SCI-Expanded)
- XXXIV. **Probing the electronic, elastic, mechanical and anisotropic features of ZrTiX<sub>4</sub> alloys via density functional theory**  
UĞUR G., Ugur S., Ozdemir A., GÜLER M., GÜLER E.  
EPL, vol.137, no.4, 2022 (SCI-Expanded)
- XXXV. **First principles study of structural, elastic, mechanical and electronic properties of nitrogen-doped cubic diamond**  
Guler E., UĞUR Ş., Guler M., Ugur G.  
Bulletin of Materials Science, vol.44, no.1, 2021 (SCI-Expanded)
- XXXVI. **A first-principles study for the elastic and mechanical properties of Ti<sub>64</sub>, Ti<sub>6242</sub> and Ti<sub>6246</sub> alloys**  
Guler E., Guler M., Ugur G., UĞUR Ş.  
EUROPEAN PHYSICAL JOURNAL B, vol.94, no.11, 2021 (SCI-Expanded)
- XXXVII. **First principles study of the electronic, optical, elastic and thermoelectric properties of Nb<sub>2</sub>WNi alloy**  
Guler M., UĞUR Ş., UĞUR G., Guler E.  
MOLECULAR PHYSICS, vol.119, no.12, 2021 (SCI-Expanded)
- XXXVIII. **First principles study of electronic, elastic, optical and magnetic properties of Rh<sub>2</sub>MnX (X = Ti, Hf, Sc, Zr, Zn) Heusler alloys**  
Guler E., Guler M., UĞUR Ş., UĞUR G.  
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, vol.121, no.10, 2021 (SCI-Expanded)
- XXXIX. **Elastic, mechanical, optical and magnetic properties of Ru<sub>2</sub>MnX (X = Nb, Ta, V) Heusler alloys**  
UĞUR Ş., Güler M., UĞUR G., Güler E.  
JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS, vol.523, 2021 (SCI-Expanded)
- XL. **Electronic structure, optical and vibrational properties of Ti<sub>2</sub>FeNiSb<sub>2</sub> and Ti<sub>2</sub>Ni<sub>2</sub>InSb double half heusler alloys**

- Ugur G., Kushwaha A. K., Guler M., Charifi Z., UĞUR Ş., Guler E., Baaziz H.  
Materials Science in Semiconductor Processing, vol.123, 2021 (SCI-Expanded)
- XLII. **Elastic, mechanical, anisotropic, optical and magnetic properties of V<sub>2</sub>NiSb Heusler alloy**  
Guler M., Guler E., UĞUR Ş., Ugur G., Charifi Z., Baaziz H.  
Physica Scripta, vol.96, no.3, 2021 (SCI-Expanded)
- XLIII. **Structural, elastic and mechanical properties of Ti-15Nb-xGe alloys: insight from DFT calculations**  
Guler E., UĞUR G., UĞUR Ş., Guler M., Khenata R.  
BULLETIN OF MATERIALS SCIENCE, vol.44, no.1, 2021 (SCI-Expanded)
- XLIV. **Elastic isotropy, magnetic and electronic properties, bonding and non-covalent interactions analyses of HoFe<sub>4</sub>P<sub>12</sub> filled-skutterudite: DFT plus U plus SOC, QTAIM and NCI investigations**  
Moussa H., Bouafia H., Sahli B., Dorbane A., UĞUR Ş., UĞUR G.  
JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS, vol.518, 2021 (SCI-Expanded)
- XLV. **Insight into the role of weak interactions on optoelectronic properties of LiGaTe 2-chalcopyrite under pressure effect: DFT-D3, NCI and QTAIM investigations**  
Bendjemai M., Bouafia H., Sahli B., Dorbane A., Ugur Ş., Ugur G., Mokrane S.  
PHYSICA B-CONDENSED MATTER, vol.599, 2020 (SCI-Expanded)
- XLVI. **First principles investigations of structural, elastic, mechanical, electronic and optical properties of triple perovskite Ba<sub>2</sub>K<sub>2</sub>Te<sub>2</sub>O<sub>9</sub>**  
Kushwaha A. K., Ugur Ş., Guler M., Guler E., Ugur G.  
PHYSICA B-CONDENSED MATTER, vol.596, 2020 (SCI-Expanded)
- XLVII. **Cation distribution effect on electronic, magnetic structure and optic properties in cobalt ferrites (Co<sub>1-y</sub>Fe<sub>y</sub>)(Tet)(Co<sub>y</sub>Fe<sub>2-y</sub>)(Oct)O<sub>4</sub> with disordered spinel structure**  
Bouferrache K., Charifi Z., Baaziz H., Ugur G., Ugur Ş., Boyacioglu B., Unver H.  
PHYSICA SCRIPTA, vol.95, no.10, 2020 (SCI-Expanded)
- XLVIII. **Ab Initio Full-Potential Study of the Structural, Electronic, and Magnetic Properties of the Cubic Sr<sub>0.75</sub>Ti<sub>0.25</sub>X(X= S, Se, and Te) Ternary Alloys**  
Hamidane N., Baaziz H., Ocak H. Y., Baddari K., Ugur Ş., Ugur G., Charifi Z.  
JOURNAL OF SUPERCONDUCTIVITY AND NOVEL MAGNETISM, vol.33, no.10, pp.3263-3272, 2020 (SCI-Expanded)
- XLIX. **A theoretical study for the band gap energies of the most common silica polymorphs**  
Guler E., Ugur G., Ugur Ş., Guler M.  
CHINESE JOURNAL OF PHYSICS, vol.65, pp.472-480, 2020 (SCI-Expanded)
- L. **Study of the ground-state magnetic ordering, magnetic and optoelectronic properties of (Lenaite) AgFeS<sub>2</sub> in its chalcopyrite structure**  
Djaafri T., Bouafia H., Sahli B., Djebour B., Ugur Ş., UĞUR G., Moussa H.  
JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS, vol.493, 2020 (SCI-Expanded)
- L. **First principles study of elastic and mechanical properties of TlBr and TlCl compounds**  
Guler M., Uğur Ş., Uğur G., Guler E.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1200, 2020 (SCI-Expanded)
- LI. **DFT-investigation on anisotropy degree of electronic, optical, and mechanical properties of olivine ZnRE<sub>2</sub>S<sub>4</sub> (RE = Er, Tm) compounds**  
Batouche M., Seddik T., Uğur Ş., Uğur G., Messekine S., Vu T. V., Khyzhun O. Y.  
MATERIALS RESEARCH EXPRESS, vol.7, no.1, 2020 (SCI-Expanded)
- LII. **Phase transitions and lattice dynamics in perovskite-type hydride Li<sub>x</sub>Na<sub>1-x</sub>MgH<sub>3</sub>**  
Karfaf S., Bennecer B., Uğur Ş., Uğur G.  
JOURNAL OF PHYSICS-CONDENSED MATTER, vol.31, no.50, 2019 (SCI-Expanded)
- LIII. **Basis set convergence of binding energy with and without CP-correction utilizing PBE0 method: A benchmark study of X-2 (X = Ge, As, Se, Sc, Ti, V, Cr, Mn, Co, Cu, Zn)**  
Akbudak S., Uğur Ş., Uğur G., Ocak H. Y.  
JOURNAL OF THEORETICAL & COMPUTATIONAL CHEMISTRY, vol.18, no.8, 2019 (SCI-Expanded)
- LIV. **Pressure effect on mechanical stability and ground state optoelectronic properties of Li<sub>2</sub>S<sub>2</sub> produced by Lithium-Sulfur batteries discharge: GGA-PBE, GLLB-SC and mBJ investigation**

Bouafia H., Sahli B., Ugur Ş., Akbudak S., UĞUR G.

PHILOSOPHICAL MAGAZINE, vol.99, no.22, pp.2789-2817, 2019 (SCI-Expanded)

- LIV. **Structural, elastic, electronic and vibrational properties of  $XAl_2O_4$  ( $X = Ca, Sr$  and  $Cd$ ) semiconductors with orthorhombic structure**  
Akbudak S., Candan A., Kushwaha A. K., Yadav A. C., UĞUR G., Ugur Ş.  
JOURNAL OF ALLOYS AND COMPOUNDS, vol.809, 2019 (SCI-Expanded)
- LVI. **First principles investigations of the structural, elastic, electronic, vibrational and thermodynamic properties of hexagonal  $XAl_2O_4$  ( $X = Cd, Ca$  and  $Sr$ )**  
Kushwaha A. K., Akbudak S., Candan A., Yadav A. C., UĞUR G., Ugur Ş.  
MATERIALS RESEARCH EXPRESS, vol.6, no.8, 2019 (SCI-Expanded)
- LVII. **Lattice dynamical and elastic properties of  $BaFX$  ( $X = Cl, Br$  and  $I$ ): Matlockite structure compounds**  
Kushwaha A. K., Akbudak S., Yadav A. C., Ugur Ş., UĞUR G.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS B, vol.33, no.20, 2019 (SCI-Expanded)
- LVIII. **Structural, elastic, electronic and thermoelectric properties of  $XPN_2$  ( $X = Li, Na$ ): First-principles study**  
Ghellab T., Baaziz H., Charifi Z., Bouferrache K., Ugur Ş., UĞUR G., Unver H.  
INTERNATIONAL JOURNAL OF MODERN PHYSICS B, vol.33, no.21, 2019 (SCI-Expanded)
- LIX. **First principles investigations of the structural, elastic, vibrational, and thermodynamic properties of  $TiMg_2O_4$  oxide spinels: cubic and tetragonal phases**  
Kushwaha A. K., Akbudak S., UĞUR G., Ugur Ş.  
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- I. **INVESTIGATION OF THE ELECTRONIC, ELASTIC, AND OPTICAL PROPERTIES OF Sc<sub>2</sub>PbZ (Z=Si, Ge, Sn) HEUSLER COMPOUNDS: FIRST-PRINCIPLES CALCULATIONS**  
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- UĞUR Ş., UĞUR G., Project Supported by Higher Education Institutions, C1b Yapıdaki Zirkonyum Tabanlı Malzemelerin Mekanik ve Dinamik Özelliklerinin DFT ile İncelenmesi, 2018 - 2019
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- UĞUR G., Project Supported by Higher Education Institutions, Bazı Nowatny-Juza bileşiklerinin yapısal, elektronik, elastik, fonon ve termodinamik özelliklerinin yoğunluk fonksiyonel teorisi ile araştırılması, 2013 - 2017
- UĞUR Ş., UĞUR G., Project Supported by Higher Education Institutions, Bazı Heusler Malzemelerin Yapısal Elastik ve Termodinamik Özelliklerinin Yoğunluk Fonksiyonel Teorisi ile İncelenmesi, 2016 - 2016
- UĞUR Ş., UĞUR G., Project Supported by Higher Education Institutions, Bazı Spinel Oksit Bileşiklerinin Yapısal Elektronik ve Titresim Özelliklerinin Ab initio Yöntemlerle İncelenmesi, 2016 - 2016
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UĞUR G., Project Supported by Higher Education Institutions, Alüminyumun Krozyon Özelliklerine Isıl ve Yüzey İşlemlerinin Etkisi, 2005 - 2007

## Tasks In Event Organizations

Uğur G., 2nd INTERNATIONAL CONGRESS ON THE WORLD OF TECHNOLOGY AND ADVANCED MATERIALS, Scientific Congress, Kırşehir, Turkey, Ekim 2016

## Metrics

Publication: 236

Citation (WoS): 1188

Citation (Scopus): 1223

H-Index (WoS): 19

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## Congress and Symposium Activities

6th International Conference on the World of Technology and Advanced Materials "WITAM'23", Invited Speaker, Batna, Algeria, 2023

## Non Academic Experience

Milli Eğitim Bakanlığı