

# **Prof. ŞULE UĞUR**

## **Personal Information**

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## **International Researcher IDs**

ScholarID: LfywhcgAAAAJ

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Publons / Web Of Science ResearcherID: B-6230-2016

ScopusID: 7004261573

Yoksis Researcher ID: 44428

## **Education Information**

Doctorate, Gazi University, Fen Bilimleri Enstitüsü, Fizik (Dr), Turkey 1996 - 2004

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

Undergraduate, Ankara University, Fen Fakültesi, Fizik Bölümü, Turkey 1983 - 1989

## **Foreign Languages**

English, B2 Upper Intermediate

## **Dissertations**

Doctorate, AIN (110) yüzeyinin atomik yapısının ve titreşim özelliklerinin yoğunluk fonksiyon teorisi ile incelenmesi, Gazi University, Fen Bilimleri Enstitüsü, Fizik (Dr), 2004

Postgraduate, Bazı anharmonik ve singüler ( $r=0$ ) potansiyeller için schrödinger denkleminin çözüm metodları, Gazi University, Fen Bilimleri Enstitüsü, Fizik (YI) (Tezli), 1994

## **Research Areas**

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, 2017 - Continues

Associate Professor, Gazi University, Fen Fakültesi, Fizik, 2010 - 2017

Assistant Professor, Gazi University, Fen Fakültesi, Fizik, 2007 - 2010

Lecturer PhD, Gazi University, Fen Fakültesi, Fizik, 2005 - 2007

## **Academic and Administrative Experience**

Birim Kalite Komisyonu Başkanı, Gazi University, Fen Fakültesi, Fizik, 2023 - Continues  
Gazi University, Fen Fakültesi, Fizik Bölümü, 2020 - Continues  
Performans Değerlendirme Komisyonu Üyesi, Gazi University, Fen Fakültesi, Fizik, 2022 - 2023  
Birim Stratejik Plan Komisyonu Üyesi, Gazi University, Fen Fakültesi, Fizik, 2021 - 2023  
Birim AR-GE ve Altyapı Komisyonu Üyesi, Gazi University, Fen Fakültesi, Fizik, 2021 - 2023  
Adaptation/Exemption Committee Member, Gazi University, Fen Fakültesi, Fizik, 2021 - 2022  
Bölüm Akademik Teşvik Değerlendirme Komisyonu Üyesi, Gazi University, Fen Fakültesi, Fizik, 2019 - 2022

## Courses

83FBE5002 YÜKSEK LİSANS TEZ ÇALIŞMASI, Postgraduate, 2023 - 2024  
83FBE5001 YÜKSEK LİSANS TEZ HAZIRLIK , Postgraduate, 2023 - 2024  
FİZ255 FİZİK LABORATUVARI (MATEMATİK BÖLÜMÜ), Undergraduate, 2023 - 2024  
FİZ251 FİZİK LABORATUVAR II (ELEKTRİK), Undergraduate, 2023 - 2024  
TERMODİNAMİK, Undergraduate, 2023 - 2024  
AKIŞKANLAR MEKANIĞI, Undergraduate, 2023 - 2024  
FİZ5048 KRİSTAL ÖRGÜ DİNAMİĞİ, Doctorate, 2022 - 2023  
FİZ2103 TİTREŞİM VE DALGALAR, Undergraduate, 2022 - 2023  
5076 İSTATİSTİK TERMODİNAMİK, Doctorate, 2022 - 2023  
FİZ3134 TERMODİNAMİK, Undergraduate, 2020 - 2021  
FİZ1126 DALGALAR VE OPTİK, Undergraduate, 2020 - 2021  
FİZ5881302 KRİSTAL ÖRGÜ DİNAMİĞİ, Doctorate, 2020 - 2021  
FİZ2123 TİTREŞİM VE DALGALAR, Undergraduate, 2021 - 2022  
FİZ5681302 İSTATİSTİK TERMODİNAMİK, Doctorate, 2020 - 2021  
FİZ2123 AKIŞKANLAR MEKANIĞI, Undergraduate, 2020 - 2021  
5341302 RADYASYON FİZİĞİNDE İSTATİSTİKSEL METODLAR, Postgraduate, 2019 - 2020  
YÜKSEK LİSANS UZMANLIK ALAN DERSİ, Postgraduate, 2017 - 2018  
FİZİK 414 ARAŞTIRMA PROJESİ II, Undergraduate, 2017 - 2018  
FİZ223 AKIŞKANLAR MEKANIĞI, Undergraduate, 2017 - 2018, 2016 - 2017  
YÜKSEK LİSANS TEZ HAZIRLIK, Postgraduate, 2017 - 2018, 2016 - 2017  
FİZİK 413 ARAŞTIRMA PROJESİ I, Undergraduate, 2017 - 2018  
FİZ5881302 KRİSTAL ÖRGÜ DİNAMİĞİ, Postgraduate, 2017 - 2018  
5950002 DOKTORA UZMANLIK ALAN DERSİ, Doctorate, 2016 - 2017  
KRİSTAL ÖRGÜ DİNAMİĞİ, Postgraduate, 2016 - 2017  
FİZ102 FİZİK II, Undergraduate, 2016 - 2017  
FİZ126 DALGALAR VE OPTİK, Undergraduate, 2015 - 2016  
FİZ154 FİZİK LAB. (Mühendislik Fak.) , Undergraduate, 2009 - 2010  
FİZ-101 GENEL FİZİK (Polatlı Fen-Edebiyat Fak.) , Undergraduate, 2010 - 2011  
FİZ-101 GENEL FİZİK (Diş Hekimliği Fak.) , Undergraduate, 2009 - 2010  
FİZ101 FİZİK-I, Undergraduate, 2005 - 2006

## Advising Theses

Uğur Ş., KÜBİK YAPIDAKİ Ti<sub>2</sub>CrZ (Z=Al, Ga, In, Si, Ge, Sn) HEUSLER ALAŞIMLARININ YAPISAL, ELEKTRONİK, ELASTİK VE OPTİK ÖZELLİKLERİNİN TEORİK OLARAK İNCELENMESİ, Postgraduate, İ.DEMİRhan(Student), 2024  
Uğur Ş., The investigation of the structural, electronic, elastic, phonon, thermodynamic and optical properties of XIn<sub>2</sub>S<sub>4</sub> (X = Mg, Zn, Cd) spinel compounds within the density functional theory, Postgraduate, Z.KIZILIRMAK(Student), 2023  
Uğur Ş., XIn<sub>2</sub>O<sub>4</sub> (X=Mg, Zn, Cd) bileşiklerinin yapışal, elektronik, elastik, fonon, termodinamik ve optik özelliklerinin teorik olarak incelenmesi, Postgraduate, S.YÜZLU(Student), 2021

UĞUR Ş., The Investigation Of Structural, Electronic, Elastic And Dynamical Properties Of Cooper To Imply Triple Heusler Compounds In Cubic Structures Within The Density Functional Theory, Postgraduate, E.ULUSU(Student), 2016

UĞUR Ş., Kübik yapıdaki Os<sub>2</sub>YPb (Y=Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn)heusler bileşiklerinin yapışal, elektronik, elastik ve titreşim özelliklerinin yoğunluk fonksiyonel teorisi ile incelenmesi, Postgraduate, S.NAZLI(Student), 2016

UĞUR Ş., Dörtlü heusler alaşımlarının yapışal, elektronik, elastik, dinamik ve termodynamik özelliklerinin yoğunluk fonksiyonel teorisi ile incelenmesi, Doctorate, A.İYİGÖR(Student), 2016

UĞUR Ş., The investigation of the structural, electronic, elastic, dynamical and thermodynamical properties of quaternary Li<sub>2</sub>XY (X=Cu,Ag,Au; Y=Ge,Sn,Sb,Al,Ga,In) compounds within the density functional theory, Postgraduate, A.KAFFASHNIA(Student), 2014

UĞUR Ş., Theoretical investigation of structural, electronic, elastic and vibrational properties of Pd<sub>2</sub>XAl (X=Co, Fe, Ni, Ti, Cu) and Pt<sub>2</sub>XAl (X=Co, Fe, Ni, Ti, Cu) heusler alloys in cubic structure, Postgraduate, A.EKİZ(Student), 2012

UĞUR Ş., The investigation of the structural, elektronik, elastic and vibrational properties of SrX (X=Se, Te) semiconductor compounds in cesium chloride structure within the density functional theory, Postgraduate, B.NAY(Student), 2011

UĞUR Ş., The investigation of structural, electronic, elastic and dynamical properties of some binary compounds in cubic structures Co<sub>Z</sub> (Z=Al, Be, Sc, Zr) within the density functional theory, Postgraduate, A.İYİGÖR(Student), 2011

UĞUR Ş., XRh (X=Mg, Sc, Y) bileşiklerinin yapışal, elektronik ve titreşimsel özelliklerinin yoğunluk fonksiyonel teorisi ile incelenmesi, Postgraduate, E.ASKER(Student), 2010

## Jury Memberships

Appointment to Academic Staff - Associate Professorship, Appointment to Academic Staff - Associate Professorship, Hakkari Üniversitesi, October, 2024

Appointment to Academic Staff-Assistant Professorship, Appointment to Academic Staff-Assistant Professorship, Gazi Üniversitesi, December, 2022

Doctorate, Doctorate, Gazi Üniversitesi, June, 2022

Appointment to Academic Staff - Associate Professorship, Appointment to Academic Staff - Associate Professorship, Gazi Üniversitesi, June, 2022

Appointment to Academic Staff-Professorship, Appointment to Academic Staff-Professorship, Gazi Üniversitesi, February, 2022

Associate Professor Exam, Associate Professor Exam, Sivas Bilim Ve Teknoloji Üniversitesi, October, 2020

PhD Thesis Monitoring Committee Member, PhD Thesis Monitoring Committee Member, Gazi Üniversitesi, June, 2020

Appointment to Academic Staff-Professorship, Appointment to Academic Staff-Professorship, Gazi Üniversitesi, February, 2020

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

### I. 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, no.11, 2024 (SCI-Expanded)

### II. 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)

### III. 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)

### IV. DFT analysis of the electronic, optical, phonon, elastic, and mechanical features of ternary Rb<sub>2</sub>XS<sub>3</sub>

- (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)
- V. 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)
- VI. DFT predictions of the electronic, phonon, optical, and thermoelectric characteristics of CaCu<sub>2</sub>S<sub>2</sub>  
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)
- VII. Unveiling the electronic, optical, and thermoelectrical properties of bulk and monolayer AlSiTe<sub>3</sub> by first principles  
GÜLER E., UĞUR Ş., GÜLER M., UĞUR G.  
CHEMICAL PHYSICS, vol.575, 2023 (SCI-Expanded)
- VIII. 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, 2023 (SCI-Expanded)
- IX. Investigating the electronic, elastic, mechanical, anisotropic, and optical aspects of Sc<sub>2</sub>RuZ (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)
- X. 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)
- XI. 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  
Baaaziz 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)
- XII. 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)
- XIII. Study of Structural, optoelectronic and elastic properties of MAX phase of Ti<sub>2</sub>BrX (X = B, C and N) by density functional theory  
Kushwaha A., Genç A., Özdemir A., Güler M., Uğur Ş.  
INORGANIC CHEMISTRY COMMUNICATIONS, vol.150, 2023 (SCI-Expanded)
- XIV. 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)
- XV. 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)
- XVI. 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)

- XVII. **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)
- XVIII. **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)
- XIX. **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)
- XX. **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)
- XXI. **<p>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((3)over bar) space group structure: Ab initio study</p>**  
 Bouafia H., UĞUR G., GÜLER M., GÜLER E., UĞUR Ş.  
 MATERIALS SCIENCE IN SEMICONDUCTOR PROCESSING, vol.146, 2022 (SCI-Expanded)
- XXII. **<p>Exploring the elastic, mechanical and anisotropic response of Ti-5Al-XSn alloys through DFT calculations</p>**  
 Guler E., UĞUR Ş., Guler M., UĞUR G.  
 CHINESE JOURNAL OF PHYSICS, vol.77, pp.151-160, 2022 (SCI-Expanded)
- XXIII. **First-principles calculations of electronic and optical properties of AgGa<sub>1-x</sub>Tl<sub>x</sub>S<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)
- XXIV. **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)
- XXV. **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)
- XXVI. **Electronic, elastic, mechanical and anisotropic response of W<sub>3</sub>XC<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)
- XXVII. **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)
- XXVIII. **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)
- XXIX. **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)

- XXX. **A first-principles study for the elastic and mechanical properties of Ti64, Ti6242 and Ti6246 alloys**

Guler E., Guler M., Ugur G., UĞUR Ş.

EUROPEAN PHYSICAL JOURNAL B, vol.94, no.11, 2021 (SCI-Expanded)

- XXXI. **A comparative study of structural, thermal, and optoelectronic properties between zircon and scheelite type structures in SrMoO<sub>4</sub> compound: An ab-initio study**

Benzineb M., Chiker F., Khachai H., Meradji H., UĞUR Ş., Naqib S., Omran S. B., Wang X., Khenata R.

OPTIK, vol.238, 2021 (SCI-Expanded)

- XXXII. **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)

- XXXIII. **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)

- XXXIV. **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)

- XXXV. **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)

- XXXVI. **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)

- XXXVII. **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)

- XXXVIII. **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)

- XXXIX. **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)

- XL. **First principles investigations of structural, elastic, mechanical, electronic and optical properties of triple perovskite Ba<sub>2</sub>K<sub>2</sub>TeO<sub>9</sub>**

Kushwaha A. K., Ugur Ş., Guler M., Guler E., Ugur G.

PHYSICA B-CONDENSED MATTER, vol.596, 2020 (SCI-Expanded)

- XLI. **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)

- XLII. **Cation distribution effect on electronic, magnetic structure and optic properties in cobalt ferrites (Co<sub>1-y</sub>Fey)(Tet)(CoyFe<sub>2-y</sub>)(Oct)O(4)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)

- XLIII. Pressure induced phase transition, electronic and optical properties of LiBeX (X = As, Sb and Bi)**  
 Guechi N., Bennecer B., Hamidani A., Uğur Ş.  
*JOURNAL OF PHYSICS-CONDENSED MATTER*, vol.32, no.32, 2020 (SCI-Expanded)
- XLIV. A theoretical study for the band gap energies of the most common silica polymorphs**  
 Guler E., Uğur G., Ugur Ş., Guler M.  
*CHINESE JOURNAL OF PHYSICS*, vol.65, pp.472-480, 2020 (SCI-Expanded)
- XLV. Study of structural, elastic, electronic, and vibrational properties of MRh<sub>2</sub>O<sub>4</sub> (M = Cd and Zn) spinels: DFT-based calculations**  
 Uğur Ş., Akbudak S., Kushwaha A. K., Bayrak G.  
*JOURNAL OF MOLECULAR MODELING*, vol.26, no.6, 2020 (SCI-Expanded)
- XLVI. 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., Uğur Ş., UĞUR G., Moussa H.  
*JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS*, vol.493, 2020 (SCI-Expanded)
- XLVII. 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)
- XLVIII. An ab-initio investigation of the electronic structure, chemical bonding and optical properties of Ba<sub>2</sub>HgS<sub>5</sub> semiconductor**  
 Azam S., Khan S. A., Khenata R., Naqib Ş., Abdiche A., Uğur Ş., Bouhemadou A., Wang X.  
*MOLECULAR PHYSICS*, vol.118, no.1, 2020 (SCI-Expanded)
- XLIX. 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)
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## Supported Projects

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- UĞUR Ş., Project Supported by Higher Education Institutions, Rh<sub>2</sub>TiAl Bileşiğinin Dinamik Özelliklerinin DFT ile İncelenmesi, 2018 - 2019
- UĞUR Ş., UĞUR G., Project Supported by Higher Education Institutions, C1b Yapıdaki Zirkonyum Tabanlı Malzemelerin Mekanik ve Dinamik Özelliklerinin DFT ile İncelenmesi, 2018 - 2019
- UĞUR Ş., Project Supported by Higher Education Institutions, A15 (Cr<sub>3</sub>Si) Tipi Yapıdaki Malzemelerin Taban Durum Özelliklerinin Ab-initio Yöntem ile İncelenmesi, 2017 - 2017
- UĞUR G., UĞUR Ş., Project Supported by Higher Education Institutions, Alüminyum tabanlı bazı üçlü intermetalik bileşiklerinin DFT ile incelenmesi, 2017 - 2017
- UĞUR Ş., TUBITAK Project, ThCr<sub>2</sub>Si<sub>2</sub> ve LuNi<sub>2</sub>B<sub>2</sub>C Tipi Süperiletkenlerin Yoğunluk Fonksiyonel Teorisi Kullanılarak İncelenmesi 114F192 ARDEB 1001, 2013 - 2017
- UĞUR Ş., UĞUR G., Project Supported by Higher Education Institutions, Bazı Heusler Malzemelerin Yapısal Elastik ve Termodinamik Özelliklerinin Yogunluk Fonksiyonel Teorisile İncelenmesi, 2016 - 2016
- UĞUR Ş., UĞUR G., Project Supported by Higher Education Institutions, Bazı Spinel Oksit Bileşiklerin Yapısal Elektronik ve Titresim Özelliklerinin Ab initio Yöntemlerle İncelenmesi, 2016 - 2016
- UĞUR Ş., UĞUR G., Project Supported by Higher Education Institutions, Ti Bazlı Üçlü Alasımının Yapısal Elektronik ve Elastik Özelliklerinin Temel Prensipler Yöntemiyle İncelenmesi, 2014 - 2016
- UĞUR Ş., UĞUR G., Project Supported by Higher Education Institutions, Bazı Kübik Kristallerin Yapısal Elektronik Elastik Özelliklerinin Teorik Olarak İncelenmesi, 2014 - 2015
- UĞUR Ş., UĞUR G., Project Supported by Higher Education Institutions, L21 Yapıdaki Heusler Bileşiklerinin Yapısal Elektronik Optik ve Termodinamik Özelliklerinin Yoğunluk Fonksiyonel Teorisi ile İncelenmesi, 2013 - 2015
- UĞUR Ş., Project Supported by Higher Education Institutions, Dörtlü Heusler Bileşiklerinin Yapısal, Elektronik, Elastik ve Titresim Özelliklerinin İncelenmesi, 2012 - 2014
- UĞUR Ş., Project Supported by Higher Education Institutions, Kübik Yapıdaki Bazı Metalik ve Yarı-Metalik Heusler Bileşiklerinin Yoğunluk Fonksiyonel Teorisi ile İncelenmesi, 2012 - 2014
- UĞUR Ş., Project Supported by Higher Education Institutions, Klinoptilolitlerin optiksel değerlendirilmesi ve dielektrik özellikleri, 2012 - 2013
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## Scientific Refereeing

## Tasks In Event Organizations

Uğur Ş., 5th International Eurasian Conference on Science, Engineering and Technology (EurasianSciEnTech 2024), Scientific Congress, Ankara, Turkey, Haziran 2024

Uğur Ş., 6th International Conference on the World of Technology and Advanced Materials "WITAM'23", Scientific Congress, Batna, Algeria, Ekim 2023

Uğur Ş., International Eurasian Conference on Science, Engineering and Technology (EurasianSciEnTech 2022), Scientific Congress, Ankara, Turkey, Aralık 2022

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## Metrics

Publication: 249

Citation (WoS): 1217

Citation (Scopus): 1256

H-Index (WoS): 19

H-Index (Scopus): 20

## Awards

Uğur Ş., GAZİ ÜNİVERSİTESİ REKTÖRLÜĞÜ TARAFINDAN 2021 ve 2022 YILINDA YAPILAN AKADEMİK YAYINLAR İÇİN AKADEMİK TEŞVİK VE ATIF ÖDÜLÜ VERİLMİŞTİR .(20.12.2023), Gazi Üniversitesi, December 2023

Uğur Ş., TÜBİTAK TEŞVİK ÖDÜLÜ, Tübitak, July 2023

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## Non Academic Experience

MİLLÎ EĞİTİM BAKANLIĞI

MİLLÎ EĞİTİM BAKANLIĞI