

Prof. GÖKAY UĞUR

Personal Information

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International Researcher IDs

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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., $Si(111)-(7 \times 7)$ 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.NİYAZI(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

- Comprehensive DFT study of $ZnGe_{1-x}SixAs_2$ alloys: Insights into structural, electronic, optical, and thermoelectric properties**
Bougaa S., Baaziz H., Ghellab T., Adalla S., Bouhdjer L., UĞUR Ş., UĞUR G., Charifi Z.

MATERIALS SCIENCE IN SEMICONDUCTOR PROCESSING, vol.188, 2025 (SCI-Expanded)

- II. **DFT+U and QTAIM insights into magnetic and optoelectronic properties, and bonding analyses of Europium-Hexafluorozirconate (EuZrF₆)**
Bouafia H., Sahli B., UĞUR G., UĞUR Ş.
Materials Chemistry and Physics, vol.332, 2025 (SCI-Expanded)
- III. **A comprehensive theoretical investigation of the structural, elastic, electronic, optical, thermal, and catalytic properties of the monoclinic perovskite ScRhO₃**
Foudia L., Reffas M., Haddadi K., Hamici M., Messalti A. S., UĞUR G.
MATERIALS SCIENCE IN SEMICONDUCTOR PROCESSING, vol.185, 2025 (SCI-Expanded)
- IV. **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)
- V. **Structural, electronic, elastic and optical properties of double spinel MgAlGaO₄: 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)
- VI. **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)
- VII. **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)
- 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, no.26, 2024 (SCI-Expanded)
- IX. **DFT analysis of the electronic, optical, phonon, elastic, and mechanical features of ternary Rb₂XS₃ (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)
- X. **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)
- XI. **Structural and mechanical investigation of a TiAl₂ based alloy: A combined theoretical and experimental study**
Mermer E., Çinici H., Uğur G., Ünal R.
MATERIALS LETTERS, vol.354, 2024 (SCI-Expanded)
- XII. **DFT predictions of the electronic, phonon, optical, and thermoelectric characteristics of CaCu₂S₂**
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)
- XIII. **Unveiling the electronic, optical, and thermoelectrical properties of bulk and monolayer AlSiTe₃ by first principles**
GÜLER E., UĞUR Ş., GÜLER M., UĞUR G.
CHEMICAL PHYSICS, vol.575, 2023 (SCI-Expanded)
- XIV. **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)

- XV. **Proposal of new stable Ru-based intermetallics, XRu_3 ($X = \text{V}, \text{Nb}$ 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)
- XVI. **Investigating the electronic, elastic, mechanical, anisotropic, and optical aspects of Sc_2RuZ ($Z: \text{Al}, \text{Ga}$, 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)
- XVII. **A theoretical benchmark for the electronic, optical, and thermoelectrical characteristics of bulk and monolayer BiS_2**
GÜLER E., UĞUR Ş., GÜLER M., UĞUR G.
MICRO AND NANOSTRUCTURES, vol.178, 2023 (SCI-Expanded)
- XVIII. **Full potential theoretical investigations for electronic, optical, mechanical, elastic and anisotropic properties of $\text{X}_2\text{Se}_2\text{C}$ ($X = \text{Ta}, \text{Nb}$) 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)
- XIX. **Properties of the double half-Heusler alloy $\text{ScNbNi}_2\text{Sn}_2$ 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)
- XX. **Experimental investigations of the structural, morphologic and mechanical properties of $\text{Ti-18 \%Nb-1.4 \%Ge}$ alloy**
Uğur G., Uğur Ş., Güler M., Güler E.
MATERIALS LETTERS, vol.335, 2023 (SCI-Expanded)
- XXI. **Revealing the electronic, optical, elastic, mechanical, anisotropic, and thermoelectric responses of $\text{Sc}(2)\text{NiZ}$ ($Z = \text{Si}, \text{Ge}$, 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)
- XXII. **Prediction of the electronic structure, optical and vibrational properties of $\text{ScXCo}_2\text{Sb}_2$ ($X = \text{V}, \text{Nb}$ 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)
- XXIII. **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)
- XXIV. **An ab initio study on phase stability, elastic and mechanical properties of Zr-doped TiAl_2 and $\alpha\text{-TiAl}_3$ intermetallics**
Mermer E., ÇİNİCİ H., UĞUR G., ÜNAL R.
EPL, vol.140, no.3, 2022 (SCI-Expanded)
- XXV. **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)
- XXVI. **Analyzing the electronic and optical properties of bulk, unstrained, and strained monolayers of SrS_2 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)
- XXVII. **Dynamical and mechanical stability, electronic properties, bonding and weak interactions analysis of new compounds MgS_2 and MgSe_2 in $\text{Pa}(\bar{3})$ 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)

- XXVIII. **The elastic, mechanical, and thermodynamic properties of NaXH₄ (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)
- XXIX. **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)
- XXX. **Structural, elastic and mechanical properties of Hf-doped TiAl₂ and alpha-TiAl₃ 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. **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)
- XXXII. **First-principles calculations of electronic and optical properties of AgGa_{1-x}TlxS₂ 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)
- XXXIII. **Probing the electronic, elastic, mechanical and anisotropic features of ZrTiX₄ alloys via density functional theory**
UĞUR G., Ugur S., Ozdemir A., GÜLER M., GÜLER E.
EPL, vol.137, no.4, 2022 (SCI-Expanded)
- XXXIV. **DFT aspects of the elastic, mechanical, magnetic, thermodynamic and optical properties of Ce₃XY perovskites**
Guler E., Guler M., UĞUR Ş., Ugur G.
PHILOSOPHICAL MAGAZINE, vol.102, no.3, pp.244-263, 2022 (SCI-Expanded)
- XXXV. **Electronic, elastic, mechanical and anisotropic response of W₃XC₂ (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)
- XXXVI. **Chemical bonding, magnetic and electronic properties, mechanical and dynamical stabilities of DyOs₄P₁₂ 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)
- XXXVII. **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)
- XXXVIII. **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)
- XXXIX. **First principles study of the electronic, optical, elastic and thermoelectric properties of Nb₂WNi alloy**
Guler M., UĞUR Ş., UĞUR G., Guler E.
MOLECULAR PHYSICS, vol.119, no.12, 2021 (SCI-Expanded)
- XL. **First principles study of electronic, elastic, optical and magnetic properties of Rh₂MnX (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)

- XLII. **Elastic, mechanical, optical and magnetic properties of Ru₂MnX (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)
- XLIII. **Electronic structure, optical and vibrational properties of Ti₂FeNiSb₂ and Ti₂Ni₂InSb 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)
- XLIV. **Elastic, mechanical, anisotropic, optical and magnetic properties of V₂NiSb Heusler alloy**
Guler M., Guler E., UĞUR Ş., Ugur G., Charifi Z., Baaziz H.
Physica Scripta, vol.96, no.3, 2021 (SCI-Expanded)
- XLV. **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)
- XLVI. **Elastic isotropy, magnetic and electronic properties, bonding and non-covalent interactions analyses of HoFe₄P₁₂ 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)
- XLVII. **Insight into the role of weak interactions on optoelectronic properties of LiGaTe₂-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)
- XLVIII. **First principles investigations of structural, elastic, mechanical, electronic and optical properties of triple perovskite Ba₂K₂Te₂O₉**
Kushwaha A. K., Ugur Ş., Guler M., Guler E., Ugur G.
PHYSICA B-CONDENSED MATTER, vol.596, 2020 (SCI-Expanded)
- XLIX. **Ab Initio Full-Potential Study of the Structural, Electronic, and Magnetic Properties of the Cubic Sr_{0.75}Ti_{0.25}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)
- L. **Cation distribution effect on electronic, magnetic structure and optic properties in cobalt ferrites (Co_{1-y}Fey)(Tet)(CoyFe_{2-y})(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)
- L. **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)
- LI. **DFT-investigation on anisotropy degree of electronic, optical, and mechanical properties of olivine ZnRE₂S₄ (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. **Study of the ground-state magnetic ordering, magnetic and optoelectronic properties of (Lenaite) AgFeS₂ 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)
- LIII. **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)
- LIV. **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. **Phase transitions and lattice dynamics in perovskite-type hydride $\text{Li}_x\text{Na}_{1-x}\text{MgH}_3$**
Karfař S., Bennecer B., Uğur Ş., Uğur G.
JOURNAL OF PHYSICS-CONDENSED MATTER, vol.31, no.50, 2019 (SCI-Expanded)
- LVI. **Pressure effect on mechanical stability and ground state optoelectronic properties of Li_2S_2 produced by Lithium-Sulfur batteries discharge: GGA-PBE, GLLB-SC and mBJ investigation**
Bouafia H., Sahli B., Uğur Ş., Akbudak S., UĞUR G.
PHILOSOPHICAL MAGAZINE, vol.99, no.22, pp.2789-2817, 2019 (SCI-Expanded)
- LVII. **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., Uğur Ş.
JOURNAL OF ALLOYS AND COMPOUNDS, vol.809, 2019 (SCI-Expanded)
- LVIII. **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., Uğur Ş.
MATERIALS RESEARCH EXPRESS, vol.6, no.8, 2019 (SCI-Expanded)
- LIX. **Lattice dynamical and elastic properties of BaFX (X = Cl, Br and I): Matlockite structure compounds**
Kushwaha A. K., Akbudak S., Yadav A. C., Uğur Ş., UĞUR G.
INTERNATIONAL JOURNAL OF MODERN PHYSICS B, vol.33, no.20, 2019 (SCI-Expanded)
- LX. **Structural, elastic, electronic and thermoelectric properties of XPN_2 (X = Li, Na): First-principles study**
Ghellab T., Baaziz H., Charifi Z., Bouferrache K., Uğur Ş., UĞUR G., Unver H.
INTERNATIONAL JOURNAL OF MODERN PHYSICS B, vol.33, no.21, 2019 (SCI-Expanded)
- LXI. **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., Uğur Ş.
JOURNAL OF MOLECULAR MODELING, vol.25, no.8, 2019 (SCI-Expanded)
- LXII. **Insight into the structural, elastic, electronic, thermoelectric, thermodynamic and optical properties of MRhSb (M = Ti, Zr, Hf) half-Heuslers from ab initio calculations**
Benzoudji F., Abid O. M., Seddik T., Yakoubi A., Khenata R., Meradji H., Uğur G., Uğur Ş., Ocak H. Y.
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- LXIII. **Thermodynamic Modeling of the Al-Ba and Ba-Ge Systems Supported by First-Principles Calculations**
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- IX. **GULP: An efficient and quick tool for molecular modelling**
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- X. **Al-1,1Sc ALAŞIMININ BAZI TERMAL ÖZELLİKLERİNİN DENEYSEL YÖNTEMLE İNCELENMESİ**
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- XI. **Al-6Mg-1,1Sc ALAŞIMININ BAZI TERMAL ÖZELLİKLERİNİN DENEYSEL YÖNTEMLE İNCELENMESİ**
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- XIV. **First Principles Study of Structural, Elastic, Electronic, Optical, Lattice Dynamical and Thermodynamical Properties of CuCr₂Se₄ Spinel**
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- XVI. **Electronic, elastic and phonon properties of LaBe₁₃ and CdBe₁₃**
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- XVIII. **On the Structural, Electronic, and Elastic Properties of Ru₂FeAl: an ab initio Study of the L₂₁ phase**
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- XX. **Elastic and optical properties of Ruddlesone-Popper perovskites-ab initio calculation**
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- XXII. **Investigations of the Core-Electron Binding Energies Using First-Principles calculations: A case study of C₂ and Sn₂**
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- XXIX. **The Thermodynamic and Vibrational Properties of Al₂Sm**
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- XXX. **Convergence of the Correlated Calculations with Correlation Energy and Total Energy: A First Principles Study**
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- XXXI. **Assesment of Resolution of Identity (RI) Method in Describing Binding Energy of Homonuclear Diatomics A Case Study of Ar₂ and H₂**
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- XXXVIII. **Ab initio investigation of the Au Sc binary system**
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- XLI. **First Principle Calculation on Structural and Lattice Dynamical Properties of LiMgSb**
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- XLII. **Electronic Structure and Optical Properties of Ruddlesden Popper Perovskite Sulfides first principle calculation**
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- XLIV. **FIRST PRINCIPLES STUDY OF STRUCTURAL ELASTIC AND THERMODYNAMIC PROPERTIES OF GeX₂O₄ X Mg Zn Cd UNDER PRESSURE**
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- XLV. **The First Principles Study on LuSe Compound in CsCl Structure**
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- XLVIII. **DENSITY FUNCTIONAL STUDY OF LuSe AND LuTe INTERMETALLIC COMPOUNDS**
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- L.V. **Kübik Spinel Yapıdaki SnX2O4 X Mg Zn Cd Bileşiklerinin Basınç Altında Termodinamik Özelliklerinin İncelenmesi**
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- L.VI. **Structural, Elastic, Electronic and Phonon Properties of SnX2O4 (X=Mg, Zn, Cd) Spinel from Density Functional Theory**
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- L.VIII. **TmX X S Se Te Bileşiklerinin Yapısal Elektronik Elastik ve Titreşim Özelliklerinin İlk Prensipler Yaklaşımı ile İncelenmesi**
CANDAN A., UĞUR G., ELLİALTIOĞLU M. R.
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- L.IX. **Kübik L21 Yapıdaki Pd2TiX X Al In Heusler Alaşımlarının Yapısal Elektronik ve Elastik Özelliklerinin İncelenmesi**
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- L.X. **Theoretical study of structural electronic and dynamical properties of B2 TiCl and TiBr**
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- L.XI. **Dy Ga Disprosiyum Galyum Bileşiklerinin Yapısal ve Elastik Özellikleri**
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- L.XII. **Pseudo potential calculations of structural elastic thermodynamic and phonon properties of spinel oxides GeX2O4 X Mg Zn Cd**
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- L.XIII. **Elastic Thermodynamical and Phonon Properties of MgIn2S4 and CdIn2S4 From First Principles Calculations**

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- LXV. **Electronic and Phonon Properties of L21 Phase Heusler Alloy Co_2CrGa**
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- LXXII. **C_{15b} Yapıdaki YMgNi_4 ve LaMgNi_4 Üçlü Bileşiklerinin Yapısal Elastik ve Elektronik Özelliklerinin İncelenmesi**
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- LXXIII. **Fe_2ScAl ve Co_2ScAl Heusler Alaşımlarının Kübik L21 Yapıdaki Elastik ve Fonon Özelliklerinin İncelenmesi**
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- LXXV. **Fe_3Si Heusler Alaşımının Yapısal Manyetik ve Elektronik Özellikleri**
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- LXXVI. **Kübik CoAl Alaşımının Elastik ve Termodinamik Özelliklerinin Hesaplanması**
İYİGÖR A., UĞUR Ş., UĞUR G., ELLİALTIOĞLU M. R.
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CANDAN A., UĞUR Ş., UĞUR G., ELLİALTIOĞLU M. R.
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- LXXXIX. **L21 Yapıdaki Ni₂FeIn heusler Bileşiğinin Titreşim Özelliklerinin Hesaplanması**
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- LXXX. **MoTa ve MoNb İkili Bileşiklerinin CsCl Yapıda Yapısal Elektronik ve Fonon Özelliklerinin İncelenmesi**
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Tasks In Event Organizations

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Citation (WoS): 1188

Citation (Scopus): 1275

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Congress and Symposium Activities

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Non Academic Experience

Milli Eğitim Bakanlığı