

## Assoc. Prof. Seçkin Dündar GÜNAY

### Personal Information

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### International Researcher IDs

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### Education Information

Doctorate, Yildiz Technical University, Fen Bilimleri, Fizik, Turkey 2002 - 2009

### Research Areas

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

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

- I. **Molecular dynamics modelling of the stress–strain response of  $\beta$ -sheet nanocrystals**  
TAŞSEVEN Ç., AKDERE Ü., GÜNAY S. D., AKSAKAL B.  
Computational Materials Science, vol.246, 2025 (SCI-Expanded)
- II. **Actinide and lanthanide dioxide lattice dilatation mechanisms with defect ingrowths**  
GÜNAY S. D.  
Journal of the American Ceramic Society, vol.106, no.6, pp.3895-3910, 2023 (SCI-Expanded)
- III. **Molecular dynamics and integral equation study of the structure and dynamics of solid and liquid magnesium phosphide**  
Aydın Y., GÜNAY S. D., AKDERE Ü., TAŞSEVEN Ç.  
Molecular Simulation, 2023 (SCI-Expanded)
- IV. **Insight into the structural, thermal and ion transport properties of solid and liquid Mg<sub>3</sub>N<sub>2</sub>: a model potential and NPT molecular dynamics simulation**  
Aydın Y., Günay S. D., AKDERE Ü., TAŞSEVEN Ç.  
MOLECULAR SIMULATION, vol.48, no.7, pp.602-609, 2022 (SCI-Expanded)
- V. **Thermophysical properties of magnesium arsenide with atomistic simulation methods**  
Günay S. D.  
Journal Of Physics And Chemistry Of Solids, vol.148, pp.1-12, 2021 (SCI-Expanded)
- VI. **Influence of repeating sequence on structural and thermal stability of crystalline domain of bombyx mori silk fibroin**  
Aksakal B., Akdere Ü., Günay S. D., Çağın T., Taşseven Ç.  
MATERIALS RESEARCH EXPRESS, vol.6, no.12, pp.125356-125364, 2020 (SCI-Expanded)
- VII. **Ordering and diffusion in liquid magnesium antimonide (Mg<sub>3</sub>Sb<sub>2</sub>) from hypernetted-chain theory and molecular dynamics simulation**

AKDERE Ü., GÜNAY S. D., TAŞSEVEN Ç.

Ionic, vol.25, no.6, pp.2711-2717, 2019 (SCI-Expanded)

VIII. **Thermal recovery mechanisms of UO<sub>2</sub> lattices by defect annihilation**

GÜNAY S. D.

JOURNAL OF ALLOYS AND COMPOUNDS, vol.724, pp.841-850, 2017 (SCI-Expanded)

IX. **Investigation of Oxygen Diffusion in Irradiated UO<sub>2</sub> with MD Simulation**

GÜNAY S. D.

HIGH TEMPERATURE MATERIALS AND PROCESSES, vol.35, no.10, pp.981-987, 2016 (SCI-Expanded)

X. **Modeling Superionic Behavior of Plutonium Dioxide**

GÜNAY S. D., AKGENC B., TAŞSEVEN Ç.

HIGH TEMPERATURE MATERIALS AND PROCESSES, vol.35, no.10, pp.999-1004, 2016 (SCI-Expanded)

XI. **Studying Static, Dynamic and Transport Properties of Mg<sub>3</sub>Bi<sub>2</sub>**

Kayadibi F., GÜNAY S. D., TAŞSEVEN Ç.

ACTA PHYSICA POLONICA A, vol.128, no.3, pp.440-446, 2015 (SCI-Expanded)

XII. **Swelling mechanisms of UO<sub>2</sub> lattices with defect ingrowths**

GÜNAY S. D.

PLoS ONE, vol.10, no.8, 2015 (SCI-Expanded)

XIII. **Hypernetted chain calculations of molten uranium dioxide: Comparison of rigid ion potentials**

GÜNAY S. D., AKDERE Ü., TAŞSEVEN Ç.

JOURNAL OF MOLECULAR LIQUIDS, vol.173, pp.124-129, 2012 (SCI-Expanded)

XIV. **THERMOPHYSICAL PROPERTIES OF URANIUM DIOXIDE: A MOLECULAR DYNAMICS STUDY OF SOLID AND LIQUID PHASES OF STOICHIOMETRIC UO<sub>2</sub>**

GÜNAY S. D., KAVANOZ H. B., AKDERE Ü., TAŞSEVEN Ç.

INTERNATIONAL JOURNAL OF MODERN PHYSICS B, vol.25, pp.3211-3223, 2011 (SCI-Expanded)

XV. **MOLECULAR DYNAMICS SIMULATION OF UO<sub>2</sub>: AN ALTERNATIVE RIGID ION MODEL POTENTIAL**

GÜNAY S. D., AKDERE Ü., KAVANOZ H. B., TAŞSEVEN Ç.

INTERNATIONAL JOURNAL OF MODERN PHYSICS B, vol.25, no.9, pp.1201-1210, 2011 (SCI-Expanded)

## Articles Published in Other Journals

I. **Calculation of thermophysical properties of magnesium antimonide alpha Mg<sub>3</sub>Sb<sub>2</sub>**

GÜNAY S. D.

Turkish Journal of Physics, vol.40, pp.264-269, 2016 (Scopus)

II. **Thermomechanical Properties of Anti-Parallel  $\beta$ -Sheets with Bombyx mori Silk Nanostructures [Gly-Ser-Gly-Ala-Gly-Ala]<sub>n</sub> and [Gly-Ala]<sub>n</sub>**

Günay S. D., Akdere Ü., Aksakal B., Çağın T., Taşseven Ç.

Materials Science Forum, vol.856, pp.74-77, 2016 (Scopus)

III. **Thermophysical Properties of Anti-Parallel  $\beta$ -Sheets with Bombyx mori Silk Nanostructures [Gly-Ser-Gly-Ala-Gly-Ala]<sub>n</sub> and [Gly-Ala]<sub>n</sub>**

Aksakal B., Günay S. D., Akdere Ü., Çağın T., Taşseven Ç.

materials science forum, vol.856, pp.70-73, 2016 (Scopus)

IV. **Classical Molecular Dynamics Simulation of Mg<sub>3</sub>Bi<sub>2</sub> at Solid and Liquid Phase**

GÜNAY S. D., Kayadibi F., Akdere Ü., Taşseven Ç.

Balkan Physics Letters, vol.15, pp.151013, 2009 (Peer-Reviewed Journal)

V. **The Structure and Ionic Transport of Liquid Semiconductor NiTe**

Akdere Ü., Günay S. D., Kavanoz H. B., Taşseven Ç.

Balkan Physics Letters, vol.15, pp.1-7, 2009 (Peer-Reviewed Journal)

VI. **Computer Simulation of Life at Low Reynolds Number**

Koltuk i. C., GÜNAY S. D.

Balkan Physics Letters - Special Issue, pp.295-297, 2007 (Peer-Reviewed Journal)

## Refereed Congress / Symposium Publications in Proceedings

- I. **THERMOPHYSICAL PROPERTIES OF NANO-CRYSTALLITE MAGNESIUM NITRIDE VIA MOLECULAR DYNAMICS SIMULATION AT CONSTANT PRESSURE**  
Aydın Y., Akdere Ü., Günay S. D., Taşseven Ç.  
TURKISH PHYSICAL SOCIETY 35 INTERNATIONAL PHYSICS CONGRESS, Muğla, Turkey, 4 - 08 September 2019, pp.351
- II. **NVE SIMULATION AND HYPERNETTED-CHAIN CALCULATION OF THE SUPERIONIC CONDUCTOR LITHIUM NITRIDE**  
Akdere Ü., Günay S. D.  
TURKISH PHYSICAL SOCIETY 35 INTERNATIONAL PHYSICS CONGRESS, Muğla, Turkey, 4 - 08 September 2019, pp.207
- III. **INTERACTION POTENTIAL AND LOCAL STRUCTURE OF LIQUID MAGNESIUM NITRIDE VIA HYPERNETTED-CHAIN THEORY**  
Aydın Y., Akdere Ü., Günay S. D., Taşseven Ç.  
TURKISH PHYSICAL SOCIETY 35 INTERNATIONAL PHYSICS CONGRESS, Muğla, Turkey, 4 - 08 September 2019, pp.342
- IV. **Static Structure and Ionic Diffusion of Liquid Magnesium Nitrate**  
AKDERE Ü., Aydın Y., GÜNAY S. D., TAŞSEVEN Ç.  
ICSEEC: SUSTAINABLE ENERGY AND ENERGY CALCULATIONS, Muğla, Turkey, 12 April 2019, pp.49
- V. **Simulation of Pullout Test on Crystallite Segment of Antiparallel beta-Sheets of Bombyx Mori Silk Fibroin**  
Uğuz C., AKDERE Ü., GÜNAY S. D., TAŞSEVEN Ç.  
ICSEEC: SUSTAINABLE ENERGY AND ENERGY CALCULATIONS, Muğla, Turkey, 12 April 2019, pp.17
- VI. **Hydrogen Bond Analysis of Bombyx Mori Silk Fibroin by MD Simulation at Room Temperature**  
Akdere Ü., Günay S. D., Taşseven Ç.  
Turkish Physical Society 34 International Physics Congress, Muğla, Turkey, 5 - 09 September 2018, pp.474
- VII. **Structural phase transition of Mg<sub>3</sub>As<sub>2</sub>**  
AKDERE Ü., GÜNAY S. D., TAŞSEVEN Ç.  
Turkish Physical Society 33rd International Physics Congress, Muğla, Turkey, 6 - 10 September 2017
- VIII. **Temperature dependence of mechanical properties of anti-parallel beta sheets with bombyx-mori silk nano structures along chain direction**  
AKDERE Ü., GÜNAY S. D., AKSAKAL B., Çağın T., TAŞSEVEN Ç.  
Turkish Physical Society 33rd International Physics Congress, Muğla, Turkey, 6 - 10 September 2017
- IX. **Molybdenum Doped CdTe Sigma<sub>3</sub>(111) Grain Boundary**  
ÇALIŞKAN M., Öztoprak A., GÜNAY S. D., TAŞSEVEN Ç., Çağın T.  
The Tenth Japanese-Mediterranean Workshop on Applied Electromagnetic Engineering for Magnetic, Superconducting, Multifunctional and Nanomaterials (JAPMED'10), İzmir, Turkey, 4 - 08 July 2017, pp.75
- X. **Polar/Antipolar - Antiparallel beta sheets of bombyx mori silk nano crystallites solvated in different type of water**  
Uğuz C., TAŞSEVEN Ç., GÜNAY S. D., AKDERE Ü.  
JAPMED 10, İzmir, Turkey, 4 - 08 July 2017
- XI. **Low- and high- temperature structural analysis of magnesium antimonide**  
GÜNAY S. D., AKDERE Ü., TAŞSEVEN Ç.  
1st International Conference on Energy and Thermal Engineering, ICTE 2017, İstanbul, Turkey, 25 - 28 April 2017
- XII. **Dynamic properties of magnesium arsenide**  
GÜNAY S. D.  
1st International Conference on Energy and Thermal Engineering, ICTE 2017, İstanbul, Turkey, 25 - 28 April 2017
- XIII. **Analysis of Mechanical Behavior of Anti Parallel Beta Sheets with Bombyx Mori Silk Nano Structures Along Inter Sheet Direction**  
Akdere Ü., Günay S. D., Aksakal B., Çağın T., Taşseven Ç.

Turkish Physical Society 32th International Physics Conference, Muğla, Turkey, 6 - 09 September 2016

- XIV. **Density functional theory study of structural and electro optical activities of grain boundaries in bi crystal CdTe**  
TAŞSEVEN Ç., ÇALIŞKAN M., GÜNAY S. D., ÇAGIN T.  
Molecular Interactions & Dynamics Gordon Research Conference, United States Of America, 10 - 15 July 2016
- XV. **Bulk property changes due to neutron irradiation in uranium dioxide**  
GÜNAY S. D.  
IMSTEC'16-Uluslararası Malzeme Bilimi ve Teknolojisi Konferansı, 6 - 08 April 2016, pp.949-950
- XVI. **Calculation of grain boundary energies of gallium arsenide with first principle study**  
GÜNAY S. D., Taşseven Ç.  
IMSTEC'16 - Uluslararası Malzeme Bilimi ve Teknolojisi Konferansı, 6 - 08 April 2016
- XVII. **Alpha particle damage in some nuclear fuels Effect on radial distribution function**  
GÜNAY S. D.  
International Conference of Computational Methods in Sciences and Engineering - ICCMSE 2016, 17 - 20 March 2016
- XVIII. **Thermomechanical properties of anti-parallel  $\beta$ -sheets with Bombyx mori silk nano structures [Gly-Ser-Gly-Ala-Gly-Ala]<sub>n</sub> and [Gly-Ala]<sub>n</sub>**  
GÜNAY S. D., AKDERE Ü., AKSAKAL B., Çağın T., TAŞSEVEN Ç.  
9th Japanese-Mediterranean Workshop on Applied Electromagnetic Engineering for Magnetic, Superconducting, Multifunctional and Nano Materials, 2015, Sofija, Bulgaria, 5 - 08 July 2015, vol.856, pp.74-77
- XIX. **Effect of Cu atoms on the band structure of CdTe**  
ÇALIŞKAN M., Öztoprak A., GÜNAY S. D., Çağın T., TAŞSEVEN Ç.  
9th Japanese-Mediterranean Workshop on Applied Electromagnetic Engineering for Magnetic, Superconducting, Multifunctional and Nano Materials, 2015, Sofija, Bulgaria, 5 - 08 July 2015, vol.856, pp.153-156
- XX. **Thermomechanical properties of anti parallel sheets with Bombyx mori silk nano structures Gly Ser Gly Ala Gly Ala n and Gly Ala n**  
Günay S. D., Akdere Ü., Aksakal B., Çağın T., Taşseven Ç.  
The Ninth Japanese -Mediterranean Workshop On Applied Electromagnetic Engineering For Magnetic,Superconducting, Multifunctional And Nanomaterials (JAPMED'9), Sofija, Bulgaria, 5 - 08 July 2015, pp.51-52
- XXI. **Thermophysical properties of anti parallel sheets with Bombyx mori silk nano structures Gly Ser Gly Ala Gly Ala n and Gly Ala n**  
Aksakal B., Günay S. D., Akdere Ü., Çağın T., Taşseven Ç.  
The Ninth Japanese -Mediterranean Workshop On Applied Electromagnetic Engineering For Magnetic,Superconducting, Multifunctional And Nanomaterials (JAPMED'9), Sofija, Bulgaria, 5 - 08 July 2015, pp.25-26
- XXII. **Thermophysical Properties of alpha-Pu2O3: A New Potential Model**  
GÜNAY Ş., Akgenc B., AKDERE Ü., TAŞSEVEN Ç.  
3rd International Congress on Advances in Applied Physics and Materials Science, Antalya, Turkey, 24 - 28 April 2013, vol.1569, pp.208-211
- XXIII. **Volume Swelling of UO2 by Irradiation of Alpha Particles and Lattice Recovery by Molecular Dynamics Simulation**  
GÜNAY S. D., KNAPP E.  
12th Granada Seminar Institute "Carlos I" for Theoretical and Computational Physics, University of Granada, Spain, 17 - 21 September 2012
- XXIV. **Monte Carlo Simulations of Polymer Brushes**  
GÜNAY S. D., Knapp E. W.  
Turkish Physical Society 28th International Physics Conference, 6 - 09 September 2011
- XXV. **HNC Calculations of Thermodynamic Properties of Molten AgI**  
GÜNAY S. D., Çalışkan M., Akdere Ü., Taşseven Ç.  
Turkish Physical Society 28th International Physics Conference, 01 September 2011

- XXVI. **A Molecular Dynamics Simulation of Premelting Effect in LiO<sub>2</sub>**  
KAYADİBİ F., GÜNAY S. D., TAŞSEVEN Ç.  
5th Nanoscience and Nanotechnology Conference (NanoTR5), Eskisehir, Turkey, Turkey, 8 - 12 June 2009
- XXVII. **Static Structure and Ionic Transport in Molten NiTe and NiTe<sub>2</sub>**  
GÜNAY S. D., Akdere Ü., Taşseven Ç.  
Turkish Physical Society 25th International Physics Conference, 25 - 29 August 2008
- XXVIII. **Observation of Steel Ball Falling Through Liquid**  
ÇELİKOK G., KOLTUK I., GÜNAY S. D.  
ISCBPU-5 5th International Student Conference of the Balkan Physical Union (ISCBPU-5), 21 - 24 August 2007
- XXIX. **Computer Simulation of Falling Object at Low Reynolds Number**  
ARŞIK A., BİLGİÖZÜ Y., PARLATAN U., GÜNAY S. D.  
4th International Student Conference of the Balkan Physical Union, 29 August - 01 September 2006
- XXX. **Equilibrium Molecular Dynamics Calculations of The Transport Properties of Molten Thallium Halides**  
GÜNAY S. D., AKDERE Ü., KOSAVALI F., TAŞSEVEN Ç.  
AIP Conference Proceedings, 22 - 26 August 2006, vol.899, pp.605
- XXXI. **The Static Structure of Liquid Semiconductors NiTe and NiTe<sub>2</sub>: Preliminary Results**  
GÜNAY S. D., Akdere Ü., Kosovalı F., Taşseven Ç.  
01 August 2006, vol.899, pp.616
- XXXII. **Study of Bose Einstein Condensation in a Harmonic Oscillator Potential**  
GÜNAY S. D., Tatlıpınar H.  
Turkish Physical Society 22th Conference, Turkey, 14 - 17 September 2004

## Supported Projects

- GÜNAY S. D., YILDIZ ŞENEL Ş., Project Supported by Higher Education Institutions, İki Boyutlu MoS<sub>2</sub>'nin Elektronik Özellikleri, 2024 - Continues
- GÜNAY S. D., AKDERE Ü., Erol A., Project Supported by Higher Education Institutions, Atomistik simülasyon yöntemleriyle ipek fibroin beta-kristal ve amorf bölgelerinin incelenmesi, 2024 - Continues
- GÜNAY S. D., Aydın Y., AKDERE Ü., TAŞSEVEN Ç., Project Supported by Higher Education Institutions, Magnezyum-Azot Grubu Bileşiklerinin Bilgisayar Simülasyonu Yöntemleriyle Fiziksel Özelliklerinin İncelenmesi, 2018 - 2020
- Aksakal B., Günay S. D., Taşseven Ç., Akdere Ü., TUBITAK Project, Yüksek performans uygulamaları için Bombyx Mori ipek fibroin kristalit biriminin termo mekaniksel özelliklerinin moleküler dinamik simülasyonu, 2016 - 2018
- TAŞSEVEN Ç., ÇALIŞKAN M., AKSAKAL B., GÜNAY S. D., Project Supported by Higher Education Institutions, Su İçerisindeki Bombyx Mori İpek Fibroinin Kristal Biriminin Termo-Mekaniksel Özelliklerinin Moleküler Dinamik Simülasyon Yöntemi ile İncelenmesi, 2015 - 2018
- Aksakal B., Taşseven Ç., Günay S. D., Akdere Ü., Çalışkan M., Project Supported by Higher Education Institutions, Su içerisindeki Bombyx Mori ipek fibroinin kristal biriminin termo mekaniksel özelliklerinin Moleküler Dinamik Simülasyon yöntemi ile incelenmesi, 2015 - 2018
- Çalışkan M., Günay S. D., Taşseven Ç., TUBITAK Project, Güneş Pillerinde Kontak Metallerinin Absorptif CdTe nin Yapısal ve Elektro Optik Aktiviteleri Üzerine Yoğunluk Fonksiyonel Teori Çalışması, 2014 - 2017
- GÜNAY S. D., Project Supported by Higher Education Institutions, Aktinit bileşenli nükleer yakıtlarda radyasyon kusurları ve geri toparlanmasının moleküler dinamik simülasyon ve SRIM ile incelenmesi, 2013 - 2016
- Akdere Ü., Taşseven Ç., GÜNAY S. D., Project Supported by Higher Education Institutions, Süperiyonik İletkenlerin Yüksek Sıcaklık Davranışları, 2003 - 2007

## Metrics

Publication: 62

Citation (WoS): 22

Citation (Scopus): 33

H-Index (WoS): 3

H-Index (Scopus): 4

### **Non Academic Experience**

FREIE ÜNİVERSİTESİ, BERLİN, ALMANYA

CHEMNITZ TEKNOLOJİ ÜNİVERSİTESİ, CHEMNİTZ, ALMANYA

TEXAS A&M ÜNİVERSİTESİ, HOUSTON, TEXAS, ABD