

## Asst. Prof. YUSUF ŞİMŞEK

### Personal Information

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### International Researcher IDs

ScholarID: 2013CjoAAAAJ

ORCID: 0000-0002-5963-2550

Publons / Web Of Science ResearcherID: AAB-4082-2021

ScopusID: 56940315200

Yoksis Researcher ID: 109060

### Education Information

Doctorate, Middle East Technical University, Graduate School Of Natural And Applied Sciences, Mikro Ve Nanoteknoloji Anabilim Dalı (Disiplinlerarası), Turkey 2008 - 2014

Postgraduate, Middle East Technical University, Graduate School Of Natural And Applied Sciences, Fizik (YI) (Tezli), Turkey 2004 - 2008

Undergraduate, Middle East Technical University, Faculty Of Arts And Sciences, Department Of Physics, Turkey 1998 - 2004

### Foreign Languages

English, C1 Advanced

### Dissertations

Doctorate, Investigation of Structural Properties of Boron Carbide Nanosystems Under Mechanical and Thermal Effects: Molecular Dynamics Simulations, Middle East Technical University, Analiz ve Fonksiyonlar Teorisi, Mikro Ve Nanoteknoloji Anabilim Dalı (Disiplinlerarası), 2014

Postgraduate, Development of software for calculations of the reflectance, transmittance and absorptance of multilayered thin films, Middle East Technical University, Analiz ve Fonksiyonlar Teorisi, Fizik (YI) (Tezli), 2008

### Research Areas

Molecular Biophysics, Atomic and Molecular Interactions

### Academic Titles / Tasks

Assistant Professor, Gazi University, Sağlık Hizmetleri Meslek Yüksekokulu, Tıbbi Hizmetler ve Teknikleri Bölümü, 2022 -

Continues

Research Assistant PhD, Gazi University, Sağlık Hizmetleri Meslek Yüksekokulu, Tıbbi Hizmetler ve Teknikleri Bölümü, 2005 - Continues

## Courses

Pozitron Emisyon Tomografisi, Associate Degree, 2022 - 2023, 2021 - 2022, 2020 - 2021, 2019 - 2020, 2018 - 2019

Spor ve Oyunların Fiziği, Undergraduate, 2021 - 2022, 2019 - 2020, 2018 - 2019

Veri Görselleştirme, Undergraduate, 2021 - 2022, 2019 - 2020, 2018 - 2019

Professional Practice, Associate Degree, 2021 - 2022, 2020 - 2021

Manyetik Rezonans Görüntüleme, Associate Degree, 2022 - 2023, 2021 - 2022, 2019 - 2020, 2018 - 2019

DOĞADA MATEMATİKSEL İLİŞKİLER, Associate Degree, 2022 - 2023

Uygulamalı Moleküler Dinamik Simülasyon, Undergraduate, 2018 - 2019

GENEL FİZİK I, Undergraduate, 2018 - 2019

MEKANİK LABORATUVARI, Undergraduate, 2018 - 2019

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

- I. **In silico identification of SARS-CoV-2 cell entry inhibitors from selected natural antivirals.**  
Şimşek Y., Baran S. S., Aslım B.  
Journal of molecular graphics & modelling, vol.109, pp.108038, 2021 (SCI-Expanded)
- II. **Two-Photon Absorption Properties of Gold Fluorescent Protein: A Combined Molecular Dynamics and Quantum Chemistry Study**  
ŞİMŞEK Y., Brown A.  
JOURNAL OF PHYSICAL CHEMISTRY B, vol.122, no.22, pp.5738-5748, 2018 (SCI-Expanded)
- III. **Structural Properties of Monolayer Boron Carbide Nanoribbons Under Strain: Molecular Dynamics Simulations**  
Simsek Y., Erkoc S.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, vol.12, no.9, pp.2180-2188, 2015 (SCI-Expanded)
- IV. **A new model for chromotherapy application**  
BAŞBINAR AKTEKİN D., ŞİMŞEK Y.  
COLOR RESEARCH AND APPLICATION, vol.37, no.2, pp.154-156, 2012 (SCI-Expanded)

## Articles Published in Other Journals

- I. **Structural Properties of Monolayer Boron Carbide Nanosheets Under Biaxial Strain Molecular Dynamics Simulations**  
ŞİMŞEK Y., ERKOÇ Ş.  
Quantum Matter, 2016 (Peer-Reviewed Journal)
- II. **Renklerin duygular üzerine etkisi**  
Başbınar Aktekin D., Şimşek Y., Kaplan B.  
Marmara tıp dergisi, vol.3, no.1, pp.31-33, 2011 (Peer-Reviewed Journal)

## Books & Book Chapters

- I. **II-VI Semiconductors Bandgap Engineering**  
KURBAN M., ŞİMŞEK Y., ERKOÇ Ş.

in: Handbook of II-VI Semiconductor-Based Sensors and Radiation Detectors, Ghenadii Korotcenkov, Editor, Springer Nature, pp.109-131, 2023

**II. Boron Carbide Nanostructures: Structural, Mechanical and Thermal Properties**

Şimşek Y., Erkoç Ş.

in: Boron Carbide: Structure, Processing, Properties and Applications, Kolan Madhav Reddy, Editor, NOVA Science Publishers Inc. , New York, pp.77-103, 2020

## **Refereed Congress / Symposium Publications in Proceedings**

- I. **Identification of Dickkopf-1/Kremen antagonist candidates using virtual screening**  
Baran S. S., Şimşek Y., Sepici Dinçel A.  
TBS INTERNATIONAL BIOCHEMISTRY CONGRESS 2023 34th NATIONAL BIOCHEMISTRY CONGRESS, Muğla, Turkey, 29 October - 01 November 2023, pp.190-191
- II. **In Silico Identification of Sclerostin Inhibitors**  
Şimşek Y., Sepici Dinçel A., Sahra Setenay B., Ergünel E., Uludamar A., Erkoç Ş.  
9th International BAU Drug Design Congress, İstanbul, Turkey, 29 November - 02 December 2023
- III. **Identification of Dickkopf-1 Antagonist Candidates Using Virtual Screening**  
Baran S. S., Şimşek Y., Sepici Dinçel A.  
9th BAU Drug Design 2023, İstanbul, Turkey, 29 November - 02 December 2023
- IV. **Two-Photon Absorption Properties of Gold Fluorescent Protein**  
ŞİMŞEK Y., Brown A.  
7th International BAU Drug Design Congress, 19 - 21 December 2019
- V. **Molecular dynamic simulation of ZP3 protein in various solutions at different temperatures**  
ŞİMŞEK Y., KOÇKAYA E. A.  
Canadian Symposium on Theoretical and Computational Chemistry, 10 - 15 July 2016
- VI. **Molecular Dynamics Simulation of ZP3 Protein in Various Solutions at Different Temperatures**  
ŞİMŞEK Y., KOÇKAYA E. A.  
27. Canadian Symposium on Theoretical and Computational Chemistry, Regina, Canada, 10 - 15 July 2016
- VII. **Compression Applications to Cubic Like Boron Carbide Nanorods Molecular Dynamics Simulations**  
ŞİMŞEK Y., NUR Y.  
Innovative Technologies in Metallurgy and Materials Science Tiflis/Gürcistan, 16 - 18 July 2015
- VIII. **Ceramic Production From Poly Silyne Co Hydridocarbyne**  
NUR Y., ŞİMŞEK Y.  
Innovative Technologies in Metallurgy and Materials Science Tiflis/Gürcistan, 16 - 18 July 2015
- IX. **Molecular Dynamics Simulations of Different Boron Carbide Nanotubes**  
ŞİMŞEK Y., NUR Y., ERKOÇ Ş.  
11. Nanobilim ve Nanateknoloji Konferansı, Turkey, 22 - 25 June 2015
- X. **Kübik Yapıdaki Bor Karbür Nano Çubuk Modelin Stres Altında Yapısal Değişimleri Moleküler Dinamik Benzeşim Teknikleri**  
ŞİMŞEK Y., ERKOÇ Ş., NUR Y.  
5. Fiziksel Kimya Kongresi, Turkey, 16 - 19 May 2015
- XI. **Molecular Dynamic Simulation of Boron Carbide Nanotubes**  
ŞİMŞEK Y., ERKOÇ Ş.  
10. Nanoscience and Nanotechnology Conference, 17 - 21 June 2014
- XII. **A Novel Approach for The Synthesis of Silicon Carbide Film**  
ŞİMŞEK Y., NUR Y.  
10. Nanoscience and Nanotechnology Conference, 17 - 21 June 2014
- XIII. **Molecular Dynamics Simulation of Graphene Like Boron Carbide Nanosheet Under Biaxial Strain**  
NUR Y., ŞİMŞEK Y.  
Bulletin of the Chemists and Technologists of Bosnia and Herzegovina Bosna Hersek, 1 - 03 January 2016

- XIV. **Synthesis of Silicon Carbide Via Sintering Poly silyne co hydridocarbyne**  
NUR Y., ŞİMŞEK Y.  
Advanced Materials World Congress (AMWC 2013), 1 - 03 January 2013
- XV. **Structural Properties of 2D Boron Carbide Sheets Under Biaxial Strain Molecular Dynamics Simulations**  
ŞİMŞEK Y., ERKOÇ Ş.  
Advanced Materials World Congress (AMWC 2013),Çeşme, 1 - 03 January 2013
- XVI. **Synthesis of SiO<sub>2</sub> Via Sintering Poly silyne co hydridocarbyne**  
NUR Y., ŞİMŞEK Y.  
International Porous and Powder Materials Symposium and Exhibition, Çeşme, 1 - 03 January 2013
- XVII. **Molecular Dynamics Simulation of Graphene Like Boron Carbide Nanoribbons Under Uniaxial Strain**  
ŞİMŞEK Y., ERKOÇ Ş.  
International Porous and Powder Materials Symposium and Exhibition, Çeşme, 1 - 03 January 2013
- XVIII. **Renk ve Duygu İlişkisi**  
Başbınar Aktekin D., Şimşek Y., Kaplan B.  
9.ulusal sinirbilimleri kongresi, İstanbul, Turkey, 13 - 17 April 2010, pp.181
- XIX. **Temel ses tonu ile depresyon ve anksiyete arasındaki ilişkisi**  
Başbınar Aktekin D., Şimşek Y., Kaplan B.  
35.ulusal fizyoloji kongresi, Ankara, Turkey, 30 September - 03 October 2009, pp.7

## Supported Projects

SEPİCİ DİNÇEL A., ŞİMŞEK Y., BARAN S. S., Project Supported by Higher Education Institutions, Sanal Tarama Yöntemleri Kullanılarak Dickkopf1 Antagonist Adaylarının Belirlenmesi, 2023 - 2024

## Scientific Refereeing

JOURNAL OF THE TURKISH CHEMICAL SOCIETY, SECTION A: CHEMISTRY, National Scientific Refreed Journal, June 2020

## Metrics

Publication: 27

Citation (WoS): 15

Citation (Scopus): 21

H-Index (WoS): 2

H-Index (Scopus): 3

## Non Academic Experience

University of Alberta, Edmonton, AB, Kanada