

## Asst. Prof. ALİ EMRE GENÇ

### Personal Information

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### International Researcher IDs

ORCID: 0000-0001-9567-2018

Yoksis Researcher ID: 134468

### Education Information

Doctorate, Gazi University, Fen Fakültesi, Fizik, Turkey 2012 - 2019

Postgraduate, Gazi University, Fen Bilimleri Enstitüsü, Fizik (YI) (Tezli), Turkey 2008 - 2011

### Foreign Languages

English, C2 Mastery

### Research Areas

Atomic and Molecular Physics, Condensed Matter 1: Structural, Mechanical and Thermal Properties, Intensive Article 2: Electronic Structure, Electric, Magnetic and Optical Properties, Computational Chemistry, Fuel Cells, Surface Chemistry, Catalysis

### Academic Titles / Tasks

Assistant Professor, Gazi University, Fen Fakültesi, Fizik, 2023 - Continues

Research Assistant PhD, Gazi University, Fen Fakültesi, Fizik, 2009 - 2023

### Courses

#### Undergraduate

Physics-Electric and Magnetism, Undergraduate, 2022 - 2023

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

- I. **Structural, electronic, elastic and optical properties of double spinel MgAlGaO<sub>4</sub>: 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)

- II. **The effect of the chemical bonding environment changes in FeNX: Hydrocarbon adsorption by DFT**  
 KÜÇÜK H., GENÇ A. E.  
*Inorganic Chemistry Communications*, vol.162, 2024 (SCI-Expanded)
- III. **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)
- IV. **Adsorption mechanism of the N<sub>2</sub> and NRR intermediates on oxygen modified MnN<sub>4</sub>-graphene layers - a single atom catalysis perspective**  
 GENÇ A. E., Tranca I.  
*Physical Chemistry Chemical Physics*, vol.25, no.27, pp.18465-18480, 2023 (SCI-Expanded)
- V. **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)
- VI. **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)
- VII. **Ammonia free catalytic reduction of nitric oxide on Ni-embedded graphene nanostructure: A density functional theory investigation**  
 GENÇ A. E., Akça A., KARAMAN C., Camarada M. B., Dragoi E.  
*Molecular Catalysis*, vol.541, 2023 (SCI-Expanded)
- VIII. **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)
- IX. **The activation of B-H bonds in borohydride on Cu(100) and Cu (110) surfaces**  
 Akça A., Genc A. E., Kutlu B.  
*COMPUTATIONAL AND THEORETICAL CHEMISTRY*, vol.1203, 2021 (SCI-Expanded)
- X. **Hydrazine decomposition on nickel-embedded graphene**  
 GENÇ A. E., KÜÇÜK H., ALP İ., Akça A.  
*INTERNATIONAL JOURNAL OF HYDROGEN ENERGY*, vol.45, no.58, pp.33407-33418, 2020 (SCI-Expanded)
- XI. **BH<sub>4</sub> dissociation on various metal (111) surfaces: A DFT study**  
 Akça A., Genc A. E., Kutlu B.  
*APPLIED SURFACE SCIENCE*, vol.473, pp.681-692, 2019 (SCI-Expanded)
- XII. **The catalytic effect of the Au(111) and Pt(111) surfaces to the sodium borohydride hydrolysis reaction mechanism: A DFT study**  
 Genc A. E., Akça A., KUTLU B.  
*INTERNATIONAL JOURNAL OF HYDROGEN ENERGY*, vol.43, no.31, pp.14347-14359, 2018 (SCI-Expanded)
- XIII. **The estimation of a (kT(C)(p)/J, p) phase diagram for a two-dimensional site-diluted Ising model using a microcanonical algorithm**  
 KUTLU B., GENÇ A. E.  
*PHYSICA A-STATISTICAL MECHANICS AND ITS APPLICATIONS*, vol.392, no.3, pp.451-457, 2013 (SCI-Expanded)

## Papers Published in Refereed Scientific Meetings

- I. **Catch the Heat!**  
 Tranca I., Shkatulov A., GENÇ A. E., KÜÇÜK H., de Boek H., Linder M., Tielens F.  
 The 19th International Conference on Density Functional Theory and its Applications (DFT2022), Brussels,

- Belgium, 28 August - 02 September 2022, pp.186
- II. **Catalytic activity Au(210) surface for sodium and Lithium borohydride hydrolysis reactions: A DFT study.**  
GENÇ A. E., AKÇA A., KUTLU B.  
International Symposium on Chemistry and Computation, İstanbul, Turkey, 30 October 2017, pp.65-66
- III. **Catalitic activity of Pt(111)and Au(111)Surface on sodium borohydride hydrolisis: a dft study**  
AKÇA A., GENÇ A. E., KUTLU B.  
TFD33, Muğla, Turkey, 6 - 10 September 2017
- IV. **dft studt of the hydroxyl ion co-adsorbtion effect on Pt(111)and Au(111) surfaces to sodium borohyride hydrolysis reaction**  
GENÇ A. E., AKÇA A., KUTLU B.  
TFD33, Muğla, Turkey, 6 September - 10 June 2017
- V. **CATALYTIC ACTIVITY OF LOW-INDEX Au(111), Au(100) AND Au(110) HIGH-INDEX Au(210) SURFACES FOR SODIUM BOROHYDRIDE HYDROLYSIS REACTION**  
GENÇ A. E., AKÇA A., KUTLU B.  
TFD33, Muğla, Turkey, 6 - 10 September 2017
- VI. **Catalysis of sodium borohydride in non catalayed solution**  
GENÇ A. E., KUTLU B.  
TURKİSH PHYSİCAL SOCIETY 32. INTERNATIONAL PHYSICS CONGRESS, 6 - 09 September 2016, vol.1, pp.134
- VII. **NaBH<sub>4</sub> Hidrolizinde Au 111 Yüzeyinin Katalitik Etkisi**  
GENÇ A. E., KUTLU B.  
21. Yoğun Madde Fiziği Ankara Toplantısı, Turkey, 25 December 2015

## Supported Projects

Genç A. E., Tranca I. C., H2020 Project, High-throughput computational screening of materials for high-temperatures heat storage, 2020 - 2021

## Metrics

Publication: 20  
Citation (WoS): 56  
Citation (Scopus): 65  
H-Index (WoS): 4  
H-Index (Scopus): 4

## Non Academic Experience

Gazi Üniversitesi Fizik Bölümü, Öğrenci Asistan