

Asst. Prof. OSMAN BARIŞ MALCIOĞLU

Personal Information

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International Researcher IDs

ScholarID: W8SFP30AAAAJ

ORCID: 0000-0003-4018-8557

Publons / Web Of Science ResearcherID: AAA-2320-2020

ScopusID: 6507506002

Yoksis Researcher ID: 294503



Education Information

2003 - 2008	Doctorate, Middle East Technical University, Graduate School of Natural and Applied Sciences, Turkey
2001 - 2003	Postgraduate, Middle East Technical University, Graduate School of Natural and Applied Sciences, Turkey
1997 - 2001	Undergraduate, Middle East Technical University, Faculty of Arts and Sciences, Department of Physics, Turkey

Foreign Languages

English, C2 Mastery Italian, B1 Intermediate French, A1 Beginner German, B1 Intermediate

Certificates, Courses and Trainings

2022	Fundamentals of Accelerated Computing with CUDA Python, IT, NVIDIA
2022	Applications of AI for Anomaly Detection , IT, NVIDIA
2022	Fundamentals of Deep Learning, IT, NVIDIA

Research Areas

Physics, Atomic and Molecular Physics, Atomic and Molecular Interactions, Molecular Properties and Interactions with Photon, Materials Science, Condensed Matter 1: Structural, Mechanical and Thermal Properties, Lattice Dynamics, Surfaces, Interfaces, Thin Films and Nanosystems, Intensive Article 2: Electronic Structure, Electric, Magnetic and Optical Properties, Electronic structure of bulk material, Electrical properties of electronic structures, interfaces, thin films and low-dimensional structures, Optical Properties, Spectroscopy of Matter, Electronic transport in condensed matter

Academic Titles / Tasks

2019 - Continues	Assistant Professor, Middle East Technical University, Faculty of Arts and Sciences, Department of Physics
2017 - 2018	Researcher, Universitaet Salzburg
2014 - 2017	Researcher, Friedrich-Alexander-Universitaet Erlangen-Nürnberg
2011 - 2014	Researcher, Université de Liège
2008 - 2010	Researcher, SISSA
2008 - 2008	Researcher, CNR Democritos
2001 - 2008	Research Assistant, Middle East Technical University, Faculty of Arts and Sciences, Department of Physics

Courses

2022 - 2023, 2021 - 2022, 2020 - 2021	INTRODUCTION TO NANOSCIENCE AND NANOTECHNOLOGY , Doctorate
2022 - 2023	GENERAL PHYSICS III , Undergraduate
2021 - 2022	PRACTICAL QUANTUM COMPUTING FOR SCIENTISTS , Undergraduate
2022 - 2023	Machine Learning with Quantum Computers, Postgraduate

Jury Memberships

September 2021	Post Graduate, Post Graduate, Orta Doğu Teknik Üniversitesi
August 2021	Post Graduate, Post Graduate, Orta Doğu Teknik Üniversitesi
September 2020	Post Graduate, Post Graduate, Orta Doğu Teknik Üniversitesi
September 2020	Post Graduate, Post Graduate, Orta Doğu Teknik Üniversitesi
October 2019	Doctorate, Doctorate, Gazi University
May 2019	Post Graduate, Post Graduate, Hacettepe Üniversitesi
May 2019	Post Graduate, Post Graduate, Orta Doğu Teknik Üniversitesi

Designed Lessons

2022 - 2023	Malcioğlu O. B., Machine Learning with Quantum Computers, Postgraduate
2021 - 2022	Malcioğlu O. B., Practical Quantum Computing for Scientists, Undergraduate

Published journal articles indexed by SCI, SSCI, and AHCI

- I. **Carbynes connected to polycyclic aromatic hydrocarbons as potential carriers of diffuse interstellar bands**
Zanolli Z., Malcioğlu O. B., Charlier J.
ASTRONOMY & ASTROPHYSICS, vol.675, 2023 (SCI-Expanded)
- II. **Self-metalation of a free-base porphyrin on a metal oxide surface mediated by extended defects: Insight from ab initio molecular dynamics simulations**
MALCIOĞLU O. B., Bockstedte M.
Surface Science, vol.723, 2022 (SCI-Expanded)
- III. **Self-metallation of a free-base porphyrin on a metal oxide surface mediated by extended defects: insight from emph{ab initio} molecular dynamics simulations**
Malcioğlu O. B., Bockstedte M.
Surface Science, no.submitted, pp.1, 2021 (SCI-Expanded)
- IV. **Morphology dependent interaction between Co(II)-tetraphenylporphyrin and the MgO(100) surface**

- Ninova S., Malcioglu O. B., Auburger P., Franke M., Lytken O., Steinrueck H., Bockstedte M.
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol.23, no.3, pp.2105-2116, 2021 (SCI-Expanded)
- V. **Effect of crystallization on the electronic and optical properties of archetypical porphyrins**
Malcioglu O. B., Bechis I., Bockstedte M.
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol.22, no.7, pp.3825-3830, 2020 (SCI-Expanded)
- VI. **Electronic structure of tetraphenylporphyrin layers on Ag(100)**
Classen A., Poeschel R., Di Filippo G., Fauster T., Malcioglu O. B., Bockstedte M.
PHYSICAL REVIEW B, vol.95, no.11, 2017 (SCI-Expanded)
- VII. **From White to Red: Electric-Field Dependent Chromaticity of Light-Emitting Electrochemical Cells based on Archetypal Porphyrins**
Weber M. D., Wittmann J. E., Burger A., Malcioglu O. B., Segarra-Marti J., Hirsch A., Coto P. B., Bockstedte M., Costa R. D.
ADVANCED FUNCTIONAL MATERIALS, vol.26, no.37, pp.6737-6750, 2016 (SCI-Expanded)
- VIII. **Structural and thermal properties of Cd-Zn-Te ternary nanoparticles: Molecular-dynamics simulations**
Kurban M., Malcioglu O. B., ERKOÇ Ş.
CHEMICAL PHYSICS, vol.464, pp.40-45, 2016 (SCI-Expanded)
- IX. **Dynamic Effect of Solvation on the Optical Properties of a CdTe Nanocrystal**
Malcioglu O. B., Raty J.
ADVANCED OPTICAL MATERIALS, vol.1, no.3, pp.239-243, 2013 (SCI-Expanded)
- X. **CdTe Nanocrystals: Dynamic Effect of Solvation on the Optical Properties of a CdTe Nanocrystal (Advanced Optical Materials 3/2013)**
MALCIOĞLU O. B., Raty J.
Advanced Optical Materials, vol.1, no.3, pp.238, 2013 (SCI-Expanded)
- XI. **Dielectric and Thermal Effects on the Optical Properties of Natural Dyes: A Case Study on Solvated Cyanin**
Malcioglu O. B., Calzolari A., Gebauer R., Varsano D., Baroni S.
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, vol.133, no.39, pp.15425-15433, 2011 (SCI-Expanded)
- XII. **turboTDDFT - A code for the simulation of molecular spectra using the Liouville-Lanczos approach to time-dependent density-functional perturbation theory**
Malcioglu O. B., Gebauer R., Rocca D., Baroni S.
COMPUTER PHYSICS COMMUNICATIONS, vol.182, no.8, pp.1744-1754, 2011 (SCI-Expanded)
- XIII. **First-principles design of efficient solar cells using two-dimensional arrays of core-shell and layered SiGe nanowires**
Pekoz R., Malcioglu O. B., Raty J. -
PHYSICAL REVIEW B, vol.83, no.3, 2011 (SCI-Expanded)
- XIV. **Harnessing molecular excited states with Lanczos chains**
Baroni S., Gebauer R., Malcioglu O. B., Saad Y., Umari P., Xian J.
JOURNAL OF PHYSICS-CONDENSED MATTER, vol.22, no.7, 2010 (SCI-Expanded)
- XV. **Initial Stages of Oxidation on Graphitic Surfaces: Photoemission Study and Density Functional Theory Calculations**
Barinov A., Malcioglu O. B., Fabris S., Sun T., Gregoratti L., Dalmiglio M., Kiskinova M.
JOURNAL OF PHYSICAL CHEMISTRY C, vol.113, no.21, pp.9009-9013, 2009 (SCI-Expanded)
- XVI. **On the Possibility of a Polymer-Like Nanorod Based on Columnar Stacked Single Benzenoid Carbon Rings**
MALCIOĞLU O. B., ERKOÇ Ş.
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, vol.6, no.4, pp.903-907, 2009 (SCI-Expanded)
- XVII. **Functionality of C(4,4) carbon nanotube as molecular detector**
MALCIOĞLU O. B., ERKOÇ Ş.
JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY, vol.8, no.2, pp.469-478, 2008 (SCI-Expanded)
- XVIII. **Structural properties of carbon nanogears**

- Tasci E., MALCIOĞLU O. B., Erkoç S.
FULLERENES NANOTUBES AND CARBON NANOSTRUCTURES, vol.16, no.1, pp.30-39, 2008 (SCI-Expanded)
- XIX. **Impact of geometry on the hydrogen storage properties of titanium carbide: a dft study on the model tic(4)h(4)**
MALCIOĞLU O. B., Erkoç S.
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, vol.18, no.12, pp.1951-1960, 2007 (SCI-Expanded)
- XX. **Thermal Stability of Carbon Nanosystems: Molecular-Dynamics Simulations**
Erkoç S., MALCIOĞLU O. B., TAŞCI E.
NANOMATERIALS: DESIGN AND SIMULATION, vol.18, pp.201-226, 2007 (SCI-Expanded)
- XXI. **Single wall bamboo shaped carbon nanotube: A molecular dynamics and electronic study**
Malcioglu O. B., Tasci E., Erkoç S.
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, vol.17, no.2, pp.187-196, 2006 (SCI-Expanded)
- XXII. **Thermal stability of benzorods: Molecular-dynamics simulations**
Malcioglu O. B., Erkoç S.
JOURNAL OF MOLECULAR GRAPHICS & MODELLING, vol.24, no.3, pp.213-218, 2005 (SCI-Expanded)
- XXIII. **Junction formation in crossed nanotubes under pressure: Molecular-dynamics simulations**
Tasci E., Malcioglu O. B., Erkoç A.
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, vol.16, no.9, pp.1371-1377, 2005 (SCI-Expanded)
- XXIV. **Structural and molecular electronic properties of B-N ring doped single-wall carbon nanotubes**
Malcioglu O. B., Tasci E., Erkoç A.
PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, vol.28, no.3, pp.296-308, 2005 (SCI-Expanded)
- XXV. **Thermal stability of Benzorod arrays: Molecular-dynamics simulations**
Malcioglu O. B., Erkoç S.
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, vol.16, no.5, pp.827-834, 2005 (SCI-Expanded)
- XXVI. **Stability of carbon nanotori under heat treatment: Molecular-dynamics simulations**
Tasci E., Yazgan E., Malcioglu O. B., Erkoç S.
FULLERENES NANOTUBES AND CARBON NANOSTRUCTURES, vol.13, no.2, pp.147-154, 2005 (SCI-Expanded)
- XXVII. **Stability of C-60 chains: molecular dynamics simulations**
Malcioglu O. B., Erkoç M.
JOURNAL OF MOLECULAR GRAPHICS & MODELLING, vol.23, no.4, pp.367-371, 2005 (SCI-Expanded)
- XXVIII. **Electronic properties of carbon nanotoroidal structures**
Yazgan E., Tasci E., Malcioglu O. B., Erkoç S.
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, vol.681, pp.231-234, 2004 (SCI-Expanded)
- XXIX. **Structural and electronic properties of single-wall GaN nanotubes: semi-empirical SCF-MO calculations**
Erkoç S., Malcioglu O. B., Tasci E.
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, vol.674, pp.1-5, 2004 (SCI-Expanded)
- XXX. **Structural and electronic properties of AlP doped Huckel type cyclacene with four benzenoid rings**
Erkoç S., Malcioglu O. B.
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, vol.14, no.9, pp.1183-1189, 2003 (SCI-Expanded)
- XXXI. **Structural properties of diamond nanorods: molecular-dynamics simulations**
Malcioglu O., Malcioglu O. B.
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, vol.14, no.4, pp.441-447, 2003 (SCI-Expanded)
- XXXII. **Structural properties of carbon nanorods: Molecular-dynamics simulations**
Erkoç S., Malcioglu O. B.
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, vol.13, no.3, pp.367-373, 2002 (SCI-Expanded)
- XXXIII. **Effect of chirality on the stability of carbon nanotubes : Molecular-dynamics simulations**
Erkoç S., Malcioglu O. B.
INTERNATIONAL JOURNAL OF MODERN PHYSICS C, vol.12, no.6, pp.865-870, 2001 (SCI-Expanded)

I. **Chapter 8 Thermal stability of carbon nanosystems: Molecular-dynamics simulations**

Erkoç Ş., MALCIOĞLU O. B., TAŞCI E.

Theoretical and Computational Chemistry, vol.18, pp.201-226, 2007 (Scopus)

Refereed Congress / Symposium Publications in Proceedings

I. **Charge State Corrections in 2d Materials Using Finite Elements**

MALCIOĞLU O. B.

NANOTR 15, 3 - 06 November 2019

II. **Structural stability of carbon nanocapsules: Molecular-dynamics simulations**

Malcioglu O. B., Tanriverdi V., Yilmaz A., Erkoc S.

Conference of the NATO-Advanced-Study-Institute on Nanoengineered Nanofibrous Materials, Belek-Antalya, Turkey, 1 - 12 September 2003, vol.169, pp.219-223

III. **Stability of carbon nanotori**

Yazgan E., Tasci E., Malcioglu O., Erkoc S.

Conference of the NATO-Advanced-Study-Institute on Nanoengineered Nanofibrous Materials, Belek-Antalya, Turkey, 1 - 12 September 2003, vol.169, pp.241-244

IV. **Simulation of carbon nanotube junction formations**

Tasci E., Malcioglu O. B., Erkoc S.

Conference of the NATO-Advanced-Study-Institute on Nanoengineered Nanofibrous Materials, Belek-Antalya, Turkey, 1 - 12 September 2003, vol.169, pp.237-240

Supported Projects

2022 - 2022

Hot electron migration in porphyrin crystals (Benchmark stage), EU Supported Other Project

Activities in Scientific Journals

2020 - Continues

Journal of the Turkish Chemical Society, Section A: Chemistry, Committee Member

Scientific Refereeing

May 2022

TUBITAK Project, 1001 - Program for Supporting Scientific and Technological Research Projects, Middle East Technical University, Turkey

March 2022

TUBITAK Project, 2209-A - Üniversite Öğrencileri Araştırma Projeleri Destekleme Programı, Yıldız Technical University, Turkey

March 2022

TUBITAK Project, 2209-A - Üniversite Öğrencileri Araştırma Projeleri Destekleme Programı, Suleyman Demirel University, Turkey

September 2021

TUBITAK Project, 2219 - Yurt Dışı Doktora Sonrası Araştırma Burs Programı, Middle East Technical University, Turkey

September 2021

TUBITAK Project, 2219 - Yurt Dışı Doktora Sonrası Araştırma Burs Programı, Middle East Technical University, Turkey

September 2021

TUBITAK Project, 2209-A - Üniversite Öğrencileri Araştırma Projeleri Destekleme Programı, Middle East Technical University, Turkey

September 2021

TUBITAK Project, 2219 - Yurt Dışı Doktora Sonrası Araştırma Burs Programı, Middle East Technical University, Turkey

July 2021

TUBITAK Project, 2209-A - Üniversite Öğrencileri Araştırma Projeleri Destekleme Programı, Middle East Technical University, Turkey

July 2021	TUBITAK Project, 2209-A - Üniversite Öğrencileri Araştırma Projeleri Destekleme Programı, Middle East Technical University, Turkey
July 2021	TUBITAK Project, 2209-A - Üniversite Öğrencileri Araştırma Projeleri Destekleme Programı, Middle East Technical University, Turkey
April 2021	TUBITAK Project, 1001 - Program for Supporting Scientific and Technological Research Projects, Middle East Technical University, Turkey
April 2021	TUBITAK Project, 1001 - Program for Supporting Scientific and Technological Research Projects, Middle East Technical University, Turkey
April 2021	TUBITAK Project, 1001 - Program for Supporting Scientific and Technological Research Projects, Middle East Technical University, Turkey
February 2021	TUBITAK Project, 2209-A - Üniversite Öğrencileri Araştırma Projeleri Destekleme Programı, Middle East Technical University, Turkey
February 2021	TUBITAK Project, 2209-A - Üniversite Öğrencileri Araştırma Projeleri Destekleme Programı, Middle East Technical University, Turkey
February 2021	TUBITAK Project, 2209-A - Üniversite Öğrencileri Araştırma Projeleri Destekleme Programı, Middle East Technical University, Turkey
February 2021	TUBITAK Project, 2209-A - Üniversite Öğrencileri Araştırma Projeleri Destekleme Programı, Middle East Technical University, Turkey
December 2020	TUBITAK Project, 2209-A - Üniversite Öğrencileri Araştırma Projeleri Destekleme Programı, Middle East Technical University, Turkey
December 2020	TÜBİTAK International Bilateral Joint Cooperation Program Project, Japan Society for the Promotion of Science, JSPS Bilateral Cooperation Program, Middle East Technical University, Turkey
December 2020	TÜBİTAK International Bilateral Joint Cooperation Program Project, Russian Foundation for Basic Research, RFBR Bilateral Cooperation Program, Middle East Technical University, Turkey
December 2020	TÜBİTAK International Bilateral Joint Cooperation Program Project, Russian Foundation for Basic Research, RFBR Bilateral Cooperation Program, Middle East Technical University, Turkey
December 2020	TUBITAK Project, 2209-A - Üniversite Öğrencileri Araştırma Projeleri Destekleme Programı, Middle East Technical University, Turkey
December 2020	TUBITAK Project, 2209-A - Üniversite Öğrencileri Araştırma Projeleri Destekleme Programı, Middle East Technical University, Turkey
December 2020	TÜBİTAK International Bilateral Joint Cooperation Program Project, Belarusian Republican Foundation for Fundamental Research, BRFFR Bilateral Cooperation Program, Middle East Technical University, Turkey
December 2020	TUBITAK Project, 1002 - Quick Support Program, Middle East Technical University, Turkey
February 2020	TUBITAK Project, 2223 - Domestic Scientific Activities Support Program, Middle East Technical University, Turkey
February 2020	TUBITAK Project, 2223 - Domestic Scientific Activities Support Program, Middle East Technical University, Turkey
January 2020	TUBITAK Project, 2219 - Yurt Dışı Doktora Sonrası Araştırma Burs Programı, Middle East Technical University, Turkey
July 2019	TÜBİTAK International Bilateral Joint Cooperation Program Project, Russian Foundation for Basic Research, RFBR Bilateral Cooperation Program, Middle East Technical University, Turkey
July 2019	TÜBİTAK International Bilateral Joint Cooperation Program Project, Russian Foundation for Basic Research, RFBR Bilateral Cooperation Program, Middle East Technical University, Turkey
February 2019	TÜBİTAK International Bilateral Joint Cooperation Program Project, Italian National Research Council, CNR Bilateral Joint Cooperation Program, Middle East Technical University, Turkey

Scientific Research / Working Group Memberships

2023 - Continues	Carbon Molecular Nanostructures In Space, https://research.iac.es/proyecto/nanospace/ , Instituto de Astrofísica de Canarias (IAC), , Spain
2020 - Continues	Romer, https://romer.metu.edu.tr , Middle East Technical University, Turkey
2019 - Continues	Günam, http://gunam.metu.edu.tr/ , Middle East Technical University, Turkey

Metrics

Publication: 39

Citation (WoS): 603

Citation (Scopus): 630

H-Index (WoS): 11

H-Index (Scopus): 11