

Prof. ALİMET SEMA ÖZEN

Personal Information

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International Researcher IDs

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Education Information

Doctorate, Bogazici University, Fen Bilimleri Enstitüsü Kimya, Turkey 1999 - 2004

Postgraduate, Bogazici University, Fen Bilimleri Enstitüsü Kimya, Turkey 1993 - 1996

Undergraduate, Bogazici University, Turkey 1987 - 1993

Research Areas

Functional Polymers, Computational Chemistry, Conductive Polymers, Composites, Quantum Mechanics, Polymeric Materials

Academic Titles / Tasks

Professor, Marmara University, Faculty of Sciences, Department of Chemistry, 2024 - Continues

Professor, Piri Reis University, Fen Edebiyat Fakültesi, 2017 - 2024

Associate Professor, Piri Reis University, Fen Edebiyat Fakültesi, 2012 - 2017

Assistant Professor, Piri Reis University, Fen Edebiyat Fakültesi, 2011 - 2012

Assistant Professor, Sabanci University, Mühendislik ve Doğa Bilimleri Fakültesi, 2008 - 2011

Lecturer, Sabanci University, Temel Geliştirme Direktörlüğü, 2004 - 2008

Research Assistant, Bogazici University, Kimya, 1993 - 1996

Academic and Administrative Experience

Faculty Management Board Member, Piri Reis University, Fen-Edebiyat Fakültesi, 2021 - 2024

Member of the Senate, Piri Reis University, Fen Edebiyat Fakültesi, 2015 - 2024

Vice Dean, Piri Reis University, Fen-Edebiyat Fakültesi, 2012 - 2016

Director of The Institution, Piri Reis University, Fen Bilimleri Enstitüsü, 2012 - 2015

Courses

Undergraduate

HSS002 Philosophy and Science, Undergraduate, 2023 - 2024

CHEM114 Chemistry, Undergraduate, 2023 - 2024

HSS019 Nanoscience and Nanotechnology, Undergraduate, 2022 - 2023

ENG 327 Introduction to Composite Structures, Undergraduate, 2017 - 2018

Published journal articles indexed by SCI, SSCI, and AHCI

- I. **Combined DFT and ionic model computational study of the effect of alkali metal cations on the structure, bonding and properties of molten cryolites, M_3AlF_6 ($M = Li, Na, K, Rb, \text{ and } Cs$)**
Özen A. S., Akdeniz Z.
Physics and Chemistry of Liquids, vol.63, no.1, pp.31-44, 2025 (SCI-Expanded)
- II. **Repetitive Rolling of Triptycene-Based Molecules on Cu Surfaces**
Konuk M., Madran M., Uysal M. T., Beşer D., Özen A. S., Akdeniz Z., Durukanoğlu S.
Journal of the American Chemical Society, vol.146, no.39, pp.27014-27021, 2024 (SCI-Expanded)
- III. **Structure and bonding in cryolitic melts a combined study by density functional theory and ionic model calculations**
Sema Özen A. S., Akdeniz Z.
Journal of Molecular Liquids, vol.368, 2022 (SCI-Expanded)
- IV. **Chemical Reactivity Perspective into the Group 2B Metals Halides**
Özen A. S., Akdeniz Z.
Journal of Physical Chemistry A, vol.120, no.25, pp.4401-4407, 2016 (SCI-Expanded)
- V. **Structure of trimers of group-2B metal dihalides from relativistic density-functional calculations**
Özen A. S., Akdeniz Z., Pastore G., Ruberto R., Tosi M.
Physics and Chemistry of Liquids, vol.53, no.1, pp.1-9, 2015 (SCI-Expanded)
- VI. **Detection of nitroaromatic explosives based on fluorescence quenching of silafluorene- and silole-containing polymers: A time-dependent density functional theory study**
Dedeoğlu B., Monari A., Etienne T., Aviyente V., Özen A. S.
Journal of Physical Chemistry C, vol.118, no.41, pp.23946-23953, 2014 (SCI-Expanded)
- VII. **Computational insight into the explosive detection mechanisms in silafluorene- and silole-containing photoluminescent polymers**
Dedeoğlu B., Aviyente V., Özen A. S.
Journal of Physical Chemistry C, vol.118, no.12, pp.6385-6397, 2014 (SCI-Expanded)
- VIII. **The origins of tetrahedral coordination in molten and glassy $ZnCl_2$ and other group-2B metal dihalides**
Özen A. S., Akdeniz Z., Ruberto R., Pastore G., Tosi M.
Physics Letters, Section A: General, Atomic and Solid State Physics, vol.378, no.4, pp.431-433, 2014 (SCI-Expanded)
- IX. **Static and dynamic structure of monomers, dimers and trimers of $HgCl_2$ from density-functional calculations**
Ruberto R., Pastore G., Özen A. S., Akdeniz Z., Tosi M.
European Physical Journal D, vol.66, no.9, 2012 (SCI-Expanded)
- X. **Peripheral and structural effects on the band gap of acceptor-donor type conducting polymers containing pendant bisfulleroid groups**
Özen A. S.
Journal of Physical Chemistry C, vol.115, no.50, pp.25007-25018, 2011 (SCI-Expanded)
- XI. **Mapping and reverse-mapping of the morphologies for a molecular understanding of the self-assembly of fluorinated block copolymers**
Kacar G., Atilgan C., Özen A. S.
Journal of Physical Chemistry C, vol.114, no.1, pp.370-382, 2010 (SCI-Expanded)
- XII. **Effect of cooperative hydrogen bonding in azo-hydrazone tautomerism of azo dyes**
Özen A. S., Doruker P., Aviyente V.
Journal of Physical Chemistry A, vol.111, no.51, pp.13506-13514, 2007 (SCI-Expanded)
- XIII. **Noncovalent intramolecular interactions in the monomers and oligomers of the acceptor and donor type of low band gap conducting polymers**

- Özen A. S., Atilgan C., Sonmez G.
Journal of Physical Chemistry C, vol.111, no.44, pp.16362-16371, 2007 (SCI-Expanded)
- XIV. **Interpretation of hydrogen bonding in the weak and strong regions using conceptual DFT descriptors**
Özen A. S., De Proft F., Aviyente V., Geerlings P.
Journal of Physical Chemistry A, vol.110, no.17, pp.5860-5868, 2006 (SCI-Expanded)
- XV. **Complete mapping of the morphologies of some linear and graft fluorinated co-oligomers in an aprotic solvent by dissipative particle dynamics**
Özen A. S., Sen U., Atilgan C.
Journal of Chemical Physics, vol.124, no.6, 2006 (SCI-Expanded)
- XVI. **A quantum mechanical approach to the kinetics of the hydrogen abstraction reaction $H_2O_2 + \cdot OH \rightarrow HO_2 + H_2O$**
Atadinç F., Günaydin H., Özen A. S., Aviyente V.
International Journal of Chemical Kinetics, vol.37, no.8, pp.502-514, 2005 (SCI-Expanded)
- XVII. **Experimental and modeling approach to decolorization of azo dyes by ultrasound: Degradation of the hydrazone tautomer**
Özen A. S., Aviyente V., Tezcanli-Güyer G., Ince N. H.
Journal of Physical Chemistry A, vol.109, no.15, pp.3506-3516, 2005 (SCI-Expanded)
- XVIII. **Modeling the substituent effect on the oxidative degradation of azo dyes**
Özen A. S., Aviyente V., De Proft F., Geerlings P.
Journal of Physical Chemistry A, vol.108, no.28, pp.5990-6000, 2004 (SCI-Expanded)
- XIX. **Modeling the oxidative degradation of azo dyes: A density functional theory study**
Özen A. S., Aviyente V., Klein R. A.
Journal of Physical Chemistry A, vol.107, no.24, pp.4898-4907, 2003 (SCI-Expanded)
- XX. **A computational study of the Wallach rearrangement**
ÖZEN A. S., ERDEM S., AVİYENTE V.
STRUCTURAL CHEMISTRY, vol.9, no.1, pp.15-25, 1998 (SCI-Expanded)

Articles Published in Other Journals

- I. **Dissolution of alumina in cryolite melts: a conceptual DFT study**
Özen A. S., Akdeniz Z.
Turkish Journal of Physics, vol.46, no.6, pp.228-238, 2022 (ESCI)

Papers Published in Refereed Scientific Meetings

- I. **Modeling Microclusters of Cryolite Melts**
ÖZEN A. S., AKDENİZ Z.
14th Chemical Physics Congress, Edirne, Turkey, 25 - 28 September 2024
- II. **QTAIM Analysis of Cryolite Clusters**
ÖZEN A. S.
26.Sivihal Sempozyumu, 22 December 2023
- III. **Electron density topology analysis within Quantum Theory of Atoms in Molecules (QTAIM) for a comprehensive understanding of local ionic states for various microclusters in Cryolitic Melts**
ÖZEN A. S., AKDENİZ Z.
İstanbul Yoğun Madde Fiziği Toplantısı, İstanbul, Turkey, 26 September 2022
- IV. **(MX₂)_n Metal Halojenür Kümelerinin Yoğunluk Fonksiyoneli Teorisi Kullanılarak İncelenmesi**
ÖZEN A. S., AKDENİZ Z.
31.Ulusal Kimya Kongresi, İstanbul, Turkey, 10 - 13 September 2019

- V. **Effect of Non-covalent Interactions on the Fluorescence Quenching Mechanism of Polymeric Sensors with Nitroaromatic Explosives**
AVIYENTE V., ÖZEN A. S., DEDEOĞLU B.
STC2018: 54th Symposium on Theoretical Chemistry, 17 - 20 September 2018
- VI. **A Computational Approach to the Explosive Detection Mechanisms in Silole- and Silafluorene Containing Photoluminescent Polymers**
ÖZEN A. S., AVIYENTE V., DEDEOĞLU B.
STC2014: 50th Symposium on Theoretical Chemistry, 14 - 18 September 2014
- VII. **Polimerlerin Patlayıcı Tespit Mekanizmalarının Modellenmesi**
ÖZEN A. S., DEDEOĞLU B., AVIYENTE V.
3. Hesaplamalı Kimya Kongresi, Turkey, 12 - 14 October 2017
- VIII. **Modeling Molecular Motors on Metal Surfaces**
ÖZEN A. S., AKDENİZ Z., madran m., DURUKANOĞLU FEYİZ M. S.
Theory and Applications of Computational Chemistry 2016, 28 August - 02 September 2016
- IX. **Explosive detection mechanisms in silole- and silafluorene containing photoluminescent polymers: a computational approach**
ÖZEN A. S., DEDEOĞLU B., AVIYENTE V.
EPF2013: European Polymer Congress, 16 - 21 June 2013
- X. **Peripheral and structural effects on the band gap of acceptor-donor type conducting polymers**
ÖZEN A. S.
EPF2013: European Polymer Congress, 16 - 21 June 2013
- XI. **Environmental and Structural Effects on the Band Gap of the Conducting Polymers with Bisfulleroid Group**
ÖZEN A. S.
ISFOE11: 4th International Symposium on Flexible Organic Electronics, 10 - 13 July 2011
- XII. **Interpretation of Hydrogen Bonding in the Weak and Strong Regions Using Conceptual DFT Descriptors**
ÖZEN A. S., AVIYENTE V.
11th International Conference on the Applications of Density Functional Theory in Chemistry and Physics, 11 - 15 September 2005
- XIII. **Mesoscopic morphologies of fluorinated oligomers in an aprotic solvent**
Şen Ü., ÖZEN A. S., Baysal C.
230th National Meeting of the American-Chemical-Society, United States Of America, 28 August - 01 September 2005, vol.230, pp.3596
- XIV. **Competing Pathways for the Oxidative Degradation of Azo Dyes**
ÖZEN A. S., AVIYENTE V.
10th International Conference on the Applications of Density Functional Theory in Chemistry and Physics, 7 - 12 September 2003
- XV. **Substituent Effect on the Oxidative Degradation of Azo Dyes**
ÖZEN A. S., AVIYENTE V.
6th World Congress of Theoretically Oriented Chemists (WATOC'02), 4 - 09 August 2002
- XVI. **Chemical Reactivity Perspective for the Oxidative Degradation of Azo Dyes**
ÖZEN A. S., AVIYENTE V.
Gordon-Kenan Chemical Physics Yaz Okulu, Gordon Research Conference, 9 - 22 September 2001

Supported Projects

Özen A. S., Akdeniz Z., TUBITAK Project, Metal Yüzeyler Üzerinde Moleküler Motorların Atomik Ölçeklerde Hareketleri, 2014 - 2017

Özen A. S., TUBITAK Project, Silol ve Silafluoren İçeren Fotolüminesan Polimerlerin Patlayıcı Maddeleri Tespit

Mekanizmalarına Hesapsal Bir Yaklaşım, 2011 - 2014

Özen A. S., Atılgan C., TUBITAK Project, Kendi Kendine Örgütlenen Moleküler Sistemlerin Dinamiğinin Çok ölçekli İncelenmesi, 2007 - 2009

Metrics

Publication: 37

Citation (WoS): 490

Citation (Scopus): 511

H-Index (WoS): 11

H-Index (Scopus): 11