

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, 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

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

SM222 Materials Science, Undergraduate, 2013 - 2014

- 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, 2024 (SCI-Expanded)
- II. **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)
- III. **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)
- IV. **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)
- V. **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)
- VI. **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)
- VII. **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)
- VIII. **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)
- IX. **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)
- X. **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)
- XI. **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)
- XII. **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)
- XIII. **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)
- XIV. **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)

- XV. **A quantum mechanical approach to the kinetics of the hydrogen abstraction reaction $H_2O_2 + \cdot OH \rightarrow H_2O + H_2O$**

Atadınç F., Günaydin H., Özen A. S., Aviyente V.

International Journal of Chemical Kinetics, vol.37, no.8, pp.502-514, 2005 (SCI-Expanded)

- XVI. **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)

- XVII. **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)

- XVIII. **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)

- XIX. **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)

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., Atilgan C., TUBITAK Project, Kendi Kendine Örgütlenen Moleküler Sistemlerin Dinamiğinin Çok ölçekli İncelenmesi, 2007 - 2009

Metrics

Publication: 20

Citation (WoS): 490

Citation (Scopus): 511

H-Index (WoS): 11

H-Index (Scopus): 11