

Assoc. Prof. İsa Değirmenci

Personal Information

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International Researcher IDs

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Publons / Web Of Science ResearcherID: H-7865-2014

ScopusID: 36950668800

Yoksis Researcher ID: 11914



Education Information

Doctorate, Bogazici University, Fen Bilimleri Enstitüsü, Kimya (Dr), Turkey 2005 - 2010

Postgraduate, Bogazici University, Fen Bilimleri Enstitüsü, Kimya (YI) (Tezli), Turkey 2002 - 2005

Undergraduate, Marmara University, Fen-Edebiyat Fakültesi, Kimya Bölümü, Turkey 1998 - 2002

Foreign Languages

English, C1 Advanced

Dissertations

Doctorate, A computational approach to the free radical polymerization of acrylates and methacrylates, Bogazici University, Fen Bilimleri Enstitüsü, Kimya (Dr), 2010

Postgraduate, Modeling the structure-reactivity relationship of acrylates, Bogazici University, Fen Bilimleri Enstitüsü, Kimya (YI) (Tezli), 2005

Research Areas

Basic Operations and Thermodynamics, Chemical Kinetics, New Technologies in Polymer Chemistry, Organic Reaction Mechanisms, Free Radicals, Natural Sciences

Academic Titles / Tasks

Assistant Professor, Ondokuz Mayıs University, Mühendislik Fakültesi, Kimya Mühendisliği Bölümü, 2013 - Continues
Research Assistant, Bogazici University, Fen-Edebiyat Fakültesi, Kimya Bölümü, 2006 - 2011

Academic and Administrative Experience

Courses

Termodinamik, Undergraduate, 2021 - 2022, 2020 - 2021, 2019 - 2020, 2018 - 2019, 2016 - 2017, 2014 - 2015, 2013 - 2014

Polimer Kimyası, Postgraduate, 2021 - 2022, 2020 - 2021, 2019 - 2020, 2018 - 2019, 2017 - 2018, 2016 - 2017

Fizikokimya, Undergraduate, 2021 - 2022, 2020 - 2021, 2019 - 2020, 2018 - 2019, 2017 - 2018, 2016 - 2017, 2014 - 2015, 2013 - 2014

Enerji Teknolojileri (SD 1), Undergraduate, 2021 - 2022, 2020 - 2021, 2019 - 2020, 2018 - 2019

Polimer Kinetiği, Postgraduate, 2020 - 2021

Polimere Giriş (SD 3), Undergraduate, 2020 - 2021, 2019 - 2020, 2018 - 2019

Mesleki İngilizce (SD 2), Undergraduate, 2020 - 2021, 2019 - 2020

Polimer Kimyası ve Teknolojisi (SD 5), Undergraduate, 2020 - 2021, 2019 - 2020, 2018 - 2019

Molekül Modellemeye Giriş, Postgraduate, 2019 - 2020, 2018 - 2019

Genel Kimya Laboratuvarı I, Undergraduate, 2019 - 2020

Kimya Mühendisliği Termodinamiği, Undergraduate, 2018 - 2019, 2017 - 2018, 2016 - 2017, 2015 - 2016, 2013 - 2014

Nükleer Enerji Reaktörleri (SD 2), Undergraduate, 2018 - 2019

Genel Kimya Laboratuvarı II, Undergraduate, 2017 - 2018

Polimere Giriş, Undergraduate, 2017 - 2018, 2016 - 2017

Mesleki İngilizce, Undergraduate, 2017 - 2018, 2016 - 2017

Polimer Kimyası ve Teknolojisi, Undergraduate, 2017 - 2018, 2016 - 2017

Enerji Teknolojileri, Undergraduate, 2017 - 2018, 2016 - 2017

ORGANİK KİMYA LABORATUVARI, Undergraduate, 2016 - 2017, 2014 - 2015, 2013 - 2014

ORGANİK KİMYA, Undergraduate, 2016 - 2017

GENEL KİMYA LABORATUVARI, Undergraduate, 2016 - 2017, 2015 - 2016, 2014 - 2015, 2013 - 2014

MOLEKÜLER MODELLEMeye GİRİŞ, Postgraduate, 2016 - 2017

Polimer Kimyası Ve Teknolojileri, Undergraduate, 2015 - 2016

Analitik Kimya Laboratuvarı, Undergraduate, 2015 - 2016, 2013 - 2014

Nükleer Enerji Reaktörleri, Undergraduate, 2015 - 2016

Analitik Kimya, Undergraduate, 2015 - 2016, 2013 - 2014

Bilgi ve İletişim Teknolojisi I, Associate Degree, 2013 - 2014

Genel Kimya, Undergraduate, 2013 - 2014

Published journal articles indexed by SCI, SSCI, and AHCI

- I. **Computational Study on Radical-Mediated Thiol-Epoxy Reactions**
Nallbani B. G., KAHRAMAN M. V., Değirmenci İ.
JOURNAL OF PHYSICAL CHEMISTRY A, vol.127, no.39, pp.8050-8058, 2023 (SCI-Expanded)
- II. **Thiol-Ene Polymerization of Natural Monomers: A DFT Study**
Mohaman H., Tuncer D., Değirmenci İ.
MACROMOLECULAR THEORY AND SIMULATIONS, vol.31, no.3, 2022 (SCI-Expanded)
- III. **Effect of Initiator Structure on Thiol-Ene Polymerization: A DFT Study**
Değirmenci İ.
MACROMOLECULAR THEORY AND SIMULATIONS, vol.31, no.1, 2022 (SCI-Expanded)
- IV. **Insight into the Thiol-yne Kinetics via a Computational Approach**
FINDIK V., Varınca B. T., Değirmenci İ., ERDEM S.
JOURNAL OF PHYSICAL CHEMISTRY A, vol.125, no.17, pp.3556-3568, 2021 (SCI-Expanded)
- V. **Solvent Effects on Thiol-Ene Kinetics and Reactivity of Carbon and Sulfur Radicals**

- Munar I., FINDIK V., Degirmenci I., AVIYENTE V.
JOURNAL OF PHYSICAL CHEMISTRY A, vol.124, no.13, pp.2580-2590, 2020 (SCI-Expanded)
- VI. **Theoretical investigation of thiol-ene click reactions: A DFT perspective**
FINDIK V., Değirmenci İ., ÇATAK Ş., AVIYENTE V.
EUROPEAN POLYMER JOURNAL, vol.110, pp.211-220, 2019 (SCI-Expanded)
- VII. **Theory and Applications of Thiyl Radicals in Polymer Chemistry**
Coote M. L., Değirmenci İ.
COMPUTATIONAL QUANTUM CHEMISTRY: INSIGHTS INTO POLYMERIZATION REACTIONS, pp.195-218, 2019 (SCI-Expanded)
- VIII. **Effect of Substituents on the Stability of Sulfur-Centered Radicals**
Değirmenci İ., Coote M. L.
JOURNAL OF PHYSICAL CHEMISTRY A, vol.120, no.37, pp.7398-7403, 2016 (SCI-Expanded)
- IX. **Comparison of Thiyl, Alkoxy, and Alkyl Radical Addition to Double Bonds: The Unusual Contrasting Behavior of Sulfur and Oxygen Radical Chemistry**
Değirmenci İ., Coote M. L.
JOURNAL OF PHYSICAL CHEMISTRY A, vol.120, no.10, pp.1750-1755, 2016 (SCI-Expanded)
- X. **First RAFT polymerization of captodative 2-acetamidoacrylic acid (AAA) monomer: An experimental and theoretical study**
Dedeoğlu B., Uğur I., Değirmenci İ., Aviyente V., Barçın B., ÇAYLI G., Acar H. Y.
POLYMER, no.19, pp.5122-5132, 2013 (SCI-Expanded)
- XI. **Origins of the solvent effect on the propagation kinetics of acrylic acid and methacrylic acid**
Değirmenci İ., Ozaltın T. F., Karahan O., Van Speybroeck V., Waroquier M., Aviyente V.
JOURNAL OF POLYMER SCIENCE PART A-POLYMER CHEMISTRY, no.9, pp.2024-2034, 2013 (SCI-Expanded)
- XII. **Controlling the tacticity in the polymerization of N-isopropylacrylamide: A computational study**
Furuncuoğlu Ö., Ozaltın T., Değirmenci İ., Aviyente V., Atlgan C., De Sterck B., Van Speybroeck V., Waroquier M.
POLYMER, no.24, pp.5503-5512, 2011 (SCI-Expanded)
- XIII. **Modeling the Solvent Effect on the Tacticity in the Free Radical Polymerization of Methyl Methacrylate**
Değirmenci İ., Eren Ş., Aviyente V., De Sterck B., Hemelsoet K., Van Speybroeck V., Waroquier M.
MACROMOLECULES, no.13, pp.5602-5610, 2010 (SCI-Expanded)
- XIV. **Role of Chain Transfer Agents in Free Radical Polymerization Kinetics**
Furuncuoğlu T., Uğur I., Değirmenci İ., Aviyente V.
MACROMOLECULES, no.4, pp.1823-1835, 2010 (SCI-Expanded)
- XV. **DFT Study on the Propagation Kinetics of Free-Radical Polymerization of α -Substituted Acrylates**
Değirmenci İ., Aviyente V., Van Speybroeck V., Waroquier M.
MACROMOLECULES, no.8, pp.3033-3041, 2009 (SCI-Expanded)
- XVI. **Efficient Free-Radical Cyclopolymerization of Oriented Styrenic Difunctional Monomers**
Edizer S., Veronesi B., Karahan O., Aviyente V., Değirmenci İ., Galbiati A., Pasini D.
MACROMOLECULES, no.6, pp.1860-1866, 2009 (SCI-Expanded)
- XVII. **Density functional theory study of free-radical polymerization of Acrylates and methacrylates: Structure-reactivity relationship**
Değirmenci İ., Avci D., Aviyente V., Van Cauter K., Van Speybroeck V., Waroquier M.
MACROMOLECULES, no.26, pp.9590-9602, 2007 (SCI-Expanded)

Articles Published in Other Journals

- I. **Role of Initiator Structure on Thiol-Ene Polymerization: A Comprehensive Theoretical Study**
Değirmenci İ.
Journal of the Turkish Chemical Society, Section A: Chemistry, vol.9, no.1, pp.149-162, 2022 (Scopus)
- II. **UNDERSTANDING THE BEHAVIOUR OF SULPHUR-CENTRED RADICALS DURING POLYMER SELF-**

HEALING

DEĞİRMENCİ İ., Coote M.

Journal of the Turkish Chemical Society, Section A: Chemistry, vol.3, no.3, pp.707-720, 2016 (Peer-Reviewed Journal)

Books & Book Chapters

I. Theory and Applications of Thiyl Radicals in Polymer Chemistry

COOTE M., DEĞİRMENCİ İ.

in: Theory and Applications of Thiyl Radicals in Polymer Chemistry, Masoud Soroush, Editor, Elsevier, pp.6-195, 2019

II. The Mechanism of Stereoregulation in Free-Radical Polymerization of Bulky Methacrylates

DEĞİRMENCİ İ., NOBLE B. B., Lin C. Y., COOTE M. L.

in: Progress in Controlled Radical Polymerization: Mechanisms and Techniques, Krzysztof Matyjaszewski, Brent S. Sumerlin, Nicolay V. Tsarevsky, Editor, American Chemical Society, pp.15-32, 2012

Refereed Congress / Symposium Publications in Proceedings

I. ROLE OF SILANES IN RADICAL POLYMERIZATION

DEĞİRMENCİ İ.

The VIII. International Istanbul Scientific Research Congress, İstanbul, Turkey, 12 - 13 March 2022

II. The Thiol-Ene Polymerization of Natural Monomers: A DFT Study

DEĞİRMENCİ İ.

III. International Joint Science Congress of Materials and Polymers (ISCM), Prishtina, Serbia, 12 - 14 September 2019

III. TAILORING THE THIOL-ENE POLYMERIZATION: A QUANTUM CHEMICAL STUDY

DEĞİRMENCİ İ.

8th International Conference on Advanced Technologies (ICAT'19), Sarajevo, Bosnia And Herzegovina, 26 - 30 August 2019

IV. TiyoL-En Reaksiyonlarında Çözücü Etkisi

MUNAR İ., DEĞİRMENCİ İ., AVİYENTE V.

31. Ulusal Kimya Kongresi, İstanbul, Turkey, 10 - 13 September 2019

V. TiyoLlerin alkinlere radikalik katılma tepkimelerinin kuramsal incelenmesi

Arslandağ İ., DEĞİRMENCİ İ.

2nd International Eurasian Conference on Biological and Chemical Sciences (EurasianBioChem 2019), Ankara, Turkey, 28 - 29 June 2019

VI. Doğal Monomerlerin TiyoL-en Tepkime Mekanizmasının Kuantum Kimyasal Yöntemlerle İncelenmesi

Mohaman H., DEĞİRMENCİ İ.

Uluslararası Katılımlı VII. PolimerBilim ve Teknoloji Kongresi, Eskişehir, Turkey, 9 - 12 September 2018

VII. Kükürt Merkezli Radikal Kimyasında Yapı-Reaktivite İlişkisinin Kuantum Kimyasal Yöntemlerle İncelenmesi

DEĞİRMENCİ İ., COOTE M.

29. Ulusal Kimya Kongresi, Ankara, Turkey, 10 - 14 September 2017

VIII. Theoretical Investigation of Thiol-Ene Click Reactions: A DFT perspective

FINDIK V., DEĞİRMENCİ İ., ÇATAK Ş., AVİYENTE V.

International Symposium on Chemistry Via Computation Applications and Molecular Nanoscience, 30 October 2017

IX. Furious and Tranquil Radicals: A Computational Study of Sulfur-Centred Radical Chemistry

DEĞİRMENCİ İ., COOTE M.

- X. **Tiyol-En Polimerizasyon Tepkimelerine π - π Etkileşimi Katkısının Kuantum Kimyasal Yöntemlerle İncelenmesi**
ERDOĞAN R., DEĞİRMENCİ İ.
29. Ulusal Kimya Kongresi, Ankara, Turkey, 10 - 14 September 2017
- XI. **Tiyol-İn ve Tiyol-En Tepkimelerinin Kuantum Mekaniksel Hesaplamalarla İncelenmesi**
YILDIZ H., DEĞİRMENCİ İ.
29. Ulusal Kimya Kongresi, Ankara, Turkey, 10 - 14 September 2017
- XII. **Understanding the Sulfur Centred Radicals Behaviour During Self Healing Mechanism**
DEĞİRMENCİ İ., Coote M.
28. Ulusal Kimya Kongresi, Mersin, Turkey, 15 - 21 August 2016
- XIII. **The Unusual Contrasting of the Same Group Element Chemical Behavior**
DEĞİRMENCİ İ., Michelle C.
MACRO 2016 - 46th IUPAC World Polymer Congress, İstanbul, Turkey, 17 - 21 July 2016
- XIV. **The Solvent Effect on the Propagation Kinetics of Acrylic Acid and Methacrylic Acid**
DEĞİRMENCİ İ., ÖZALTIN T. F., KARAHAN Ö., AVİYENTE V.
44th IUPAC World Chemistry Congress, İstanbul, Turkey, 11 - 16 August 2013
- XV. **Structure Reactivity Relationship of Alpha Substituted Acrylates**
DEĞİRMENCİ İ., Lin C. Y., COOTE M., AVİYENTE V.
The 32nd Australasian Polymer Symposium (32APS), Coffs Harbour, Australia, 13 February 2013
- XVI. **Effect of Solvent on tacticity control of methyl methacrylate polymerization A DFT Study**
DEĞİRMENCİ İ., Eren Ş., AVİYENTE V., De Sterck B., Hemelsoet K., Van Speybroeck V., Waroquier M.
The European Polymer Congress, Graz, Austria, 12 - 17 July 2009
- XVII. **How does the chain length affect the kinetics of free radical polymerization of alpha substituted acrylates**
DEĞİRMENCİ İ., AVİYENTE V., Van Speybroeck V., Waroquier M.
6th Congress on Electronic Structure: Principles and Applications (ESPA), Palma De Mallorca, Spain, 2 - 05 September 2008
- XVIII. **How does the chain length affect the kinetics of free radical polymerization of methylacrylate**
Eren Ş., DEĞİRMENCİ İ., AVİYENTE V.
8th International Chemical Physics Congress, İstanbul, Turkey, 24 - 25 April 2008
- XIX. **DFT study of free radical polymerization of a substituted acrylates chain length dependence on the propagation rate constant**
DEĞİRMENCİ İ., AVİYENTE V.
8th International Chemical Physics Congress, İstanbul, Turkey, 24 - 25 April 2008
- XX. **Modeling the Cyclopolymerization of Difunctional Monomers**
KARAHAN Ö., Edizer S., DEĞİRMENCİ İ., AVİYENTE V., Pasini D.
8th International Chemical Physics Congress, İstanbul, Turkey, 24 - 25 April 2008
- XXI. **Modeling the propagation kinetics of the free radical polymerization of methylmethacrylate**
ŞILDIR H., DEĞİRMENCİ İ., AVİYENTE V.
8th International Chemical Physics Congress, İstanbul, Turkey, 24 - 25 April 2008
- XXII. **Role of Chain Transfer in the Free Radical Polymerization of Ethylene**
DEĞİRMENCİ İ., AVİYENTE V.
12th International Conference on the Applications of Density Functional Theory, Amsterdam, Netherlands, 26 - 30 August 2007
- XXIII. **The Effect of Capto dative Substitution on Free Radical Polymerization for Acrylate Monomers**
İnçmen M., DEĞİRMENCİ İ., AVCI SEMİZ D., AVİYENTE V.
4th IUPAC sponsored International Symposium on Radical Polymerization: Kinetics and Mechanism Scientific Meeting, Il Ciocco, Italy, 03 September 2006
- XXIV. **Effect of Chain Transfer on the Free Radical Polymerization of Acrylates A Computational Study**
DEĞİRMENCİ İ., AVCI SEMİZ D., AVİYENTE V.

International 7th Chemical Physics Congress, Isparta, Turkey, 19 - 20 May 2006

XXV. Modeling the Reactivity Structure Relationship of Acrylates

DEĞİRMENCİ İ., AVCI SEMİZ D., AVİYENTE V.

The 11th International Conference on the Applications of Density Functional Theory in Chemistry and Physics, Cenevre, Switzerland, 11 - 15 September 2005, vol.59

XXVI. Modeling the Reactivity of New Phosphorus Containing Acrylates

DEĞİRMENCİ İ., SALMAN S., AVCI SEMİZ D., AVİYENTE V.

6th International Conference on Chemical Physics, İstanbul, Turkey, 15 - 17 October 2004

Supported Projects

Değirmenci İ., Tiyol-En Tepkimelerinde Yapı-Reaktivite İlişkisinin Kuantum Mekaniksel Yöntemlerle İncelenmesi, 2018 - 2020

Scientific Refereeing

RSC ADVANCES, Journal Indexed in SCI-E, July 2023

CHEMISTRYSELECT, Journal Indexed in SCI-E, January 2023

TURKISH JOURNAL OF CHEMISTRY, National Scientific Refreed Journal, August 2022

CHEMISTRYSELECT, Journal Indexed in SCI-E, August 2022

NATURE CHEMISTRY, Journal Indexed in SCI-E, August 2021

JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, Journal Indexed in SCI-E, December 2019

Journal of the Turkish Chemical Society, Section A: Chemistry, National Scientific Refreed Journal, October 2018

JOURNAL OF MOLECULAR MODELING, Journal Indexed in SCI-E, May 2017

JOURNAL OF THEORETICAL AND COMPUTATIONAL CHEMISTRY, Journal Indexed in SCI-E, January 2017

JOURNAL OF THEORETICAL AND COMPUTATIONAL CHEMISTRY, Journal Indexed in SCI-E, September 2016

MACROMOLECULAR THEORY AND SIMULATIONS, Journal Indexed in SCI-E, December 2014

Metrics

Publication: 47

Citation (WoS): 496

Citation (Scopus): 509

H-Index (WoS): 11

H-Index (Scopus): 11

Scholarships

Thiuram Disulfit (TDS) İçeren Polimerlerin Kendi Kendine İyileşme Mekanizmasının İncelenmesi, TÜBİTAK, 2015 - 2016

Non Academic Experience

Australian National University

Australian National University