

## Prof. YAVUZ DEDE

### Personal Information

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### International Researcher IDs

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Publons / Web Of Science ResearcherID: AIC-4285-2022

ScopusID: 26026920900

Yoksis Researcher ID: 137346

### Education Information

Post Doctorate, Indiana University at Bloomington, Department of Chemistry, United States Of America 2008 - 2009

Doctorate, Middle East Technical University, Faculty Of Arts And Sciences, Department Of Chemistry, Turkey 2002 - 2007

Postgraduate, Middle East Technical University, Faculty Of Arts And Sciences, Department Of Chemistry, Turkey 1999 - 2002

Undergraduate, Ihsan Dogramaci Bilkent University, Faculty Of Science, Department Of Chemistry, Turkey 1995 - 1999

### Dissertations

Doctorate, Quantum chemical investigation of reactions of atomic carbon with water and methanol, Middle East Technical University, Analiz ve Fonksiyonlar Teorisi, Kimya (Dr), 2007

Postgraduate, Supramolecules for constructing nanoscale devices, Middle East Technical University, Analiz ve Fonksiyonlar Teorisi, Kimya (YI) (Tezli), 2002

### Research Areas

Chemistry, Physical Chemistry, Computational Chemistry, Chemical Kinetics, Quantum Mechanics, Transition Metals, Photochemistry of Inorganic Molecules, Inorganic Reaction Mechanisms and Kinetics, Catalysis, Coordination Chemistry, Organometallic Chemistry, Chemistry of Dyes and Pigments, Natural Sciences

### Academic Titles / Tasks

Professor, Gazi University, Fen Fakültesi, Kimya, 2022 - Continues

Associate Professor, Gazi University, Fen Fakültesi, Kimya, 2014 - 2022

Lecturer PhD, Gazi University, Fen Fakültesi, Kimya, 2010 - 2014

### Advising Theses

DEDE Y., Active Center Design Of Non-Heme Enzymes Based On Secondary Sphere Effects, Postgraduate,

M.BÜYÜKTEMİZ(Student), 2020

DEDE Y., Co(IV)-okso merkezinde O-O bağ oluşumunun kuantum kimyasal incelenmesi, Postgraduate,

U.ŞAHİN(Student), 2020

DEDE Y., Quantum Chemical Investigation Of Electronic Structure Of The Janus Green Dye, Postgraduate,

D.BERNA(Student), 2020

DEDE Y., Non-heme enzimlerde ikincil koordinasyon küresi etkilerini temel alarak yeni aktif merkezlerin modellenmesi,

Postgraduate, M.BÜYÜKTEMİZ(Student), 2020

DEDE Y., Oxidative Methane Activation With Cationic Ligand - Metal Complexes, Postgraduate, Y.OCAK(Student), 2020

DEDE Y., Quantum Chemical Analysis Of O-O Bond Formation At Co(Iv)-Oxo Center, Postgraduate, U.ŞAHİN(Student), 2020

DEDE Y., Quantum Chemical Investigation Of O-O And C-C Bond Activation Reactions Of Homoprotocatechuate 2,3-Dioxygenase Active Site Complex, Postgraduate, S.YALÇIN(Student), 2015

DEDE Y., Ni merkezli geçiş metali kompleksleri ile oksijen aktivasyonu mekanizmalarının kuantum kimyasal incelenmesi, Postgraduate, G.ALICI(Student), 2012

DEDE Y., Quantum chemical investigation of electronic structure of boron di-pyrromethene fluorophores with multi-reference (MCSCF) methods, Postgraduate, S.DUMAN(Student), 2012

DEDE Y., Quantum chemical investigation of dioxygen activation by Ni-bearing transition metal complexes, Postgraduate, G.Alıcı(Student), 2012

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

- I. **Phthalocyanine vs porphyrin: Experimental and theoretical comparison of the catalytic activity of N-bridged diiron tetrapyrrolic complexes for alcohols oxidation**  
ŞAHİN Z., Yüceel Ç., Yıldız D. B., DEDE Y., DUMOULIN F., İŞÇİ Ü.  
Molecular Catalysis, vol.559, 2024 (SCI-Expanded)
- II. **Homoprotocatechuate dioxygenase active site: Imitating the secondary sphere base via computational design**  
BÜYÜKTEMİZ M., DEDE Y.  
Turkish Journal of Chemistry, vol.47, no.5, pp.1116-1124, 2023 (SCI-Expanded)
- III. **The Role of the Redox Non-Innocent Hydroxyl Ligand in the Activation of O<sub>2</sub> Performed by [Ni(H)(OH)].**  
Kim J., Büyüktemiz M., Alıcı G., Baik M., Dede Y.  
CHEMISTRY - A EUROPEAN JOURNAL, vol.2022, 2022 (SCI-Expanded)
- IV. **Substitution effects in distyryl BODIPYs for near infrared organic photovoltaics**  
Tok M., Say B., Dolek G., Tatar B., Özgür D., Kurukavak C. K., Kuş M., Dede Y., Cakmak Y.  
JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY, vol.429, 2022 (SCI-Expanded)
- V. **Light-Driven Water Oxidation with Ligand-Engineered Prussian Blue Analogues**  
Ahmad A. A., Ghobadi T. G. U., BÜYÜKTEMİZ M., ÖZBAY E., DEDE Y., KARADAŞ F.  
INORGANIC CHEMISTRY, vol.61, no.9, pp.3931-3941, 2022 (SCI-Expanded)
- VI. **Building an Iron Chromophore Incorporating Prussian Blue Analogue for Photoelectrochemical Water Oxidation**  
Ghobadi T. G. U., Ghobadi A., Demirtas M., BÜYÜKTEMİZ M., Ozvural K. N., YILDIZ E., Erdem E., YAĞLIOĞLU H. G., DURGUN E., DEDE Y., et al.  
CHEMISTRY-A EUROPEAN JOURNAL, vol.27, no.35, pp.8966-8976, 2021 (SCI-Expanded)
- VII. **When Does Fusing Two Rings Not Yield a Larger Ring? The Curious Case of BOPHY**  
BÜYÜKTEMİZ M., Kilic M., Che Y., Zhao J., DEDE Y.  
JOURNAL OF ORGANIC CHEMISTRY, vol.86, no.6, pp.4547-4556, 2021 (SCI-Expanded)
- VIII. **Excited state structures projected onto two dimensions: correlations with luminescent behavior**  
DEDE Y., Yalcin S., BÜYÜKTEMİZ M.  
JOURNAL OF MATHEMATICAL CHEMISTRY, vol.58, no.10, pp.2254-2272, 2020 (SCI-Expanded)

- IX. **The Role of Molecular Structure of Phenylalanine Peptides on the Formation of Vertically Aligned Ordered Bionanostructures: Implications for Sensing Application**  
Sahibbeyli V., Yildiz D. B., Papir G., DEDE Y., DEMİREL G.  
ACS APPLIED NANO MATERIALS, vol.3, no.5, pp.4305-4313, 2020 (SCI-Expanded)
- X. **A Robust, Precious-Metal-Free Dye-Sensitized Photoanode for Water Oxidation: A Nanosecond-Long Excited State Lifetime through a Prussian Blue Analogue**  
Ghobadi T. G. U., Ghobadi A., BÜYÜKTEMİZ M., YILDIZ E., Yildiz D. B., YAĞLIOĞLU H. G., DEDE Y., ÖZBAY E., KARADAŞ F.  
ANGEWANDTE CHEMIE-INTERNATIONAL EDITION, vol.59, no.10, pp.4082-4090, 2020 (SCI-Expanded)
- XI. **Control of triboelectric charges on common polymers by photoexcitation of organic dyes**  
Cezan S. D., Nalbant A. A., BÜYÜKTEMİZ M., DEDE Y., BAYTEKİN H. T., BAYTEKİN B.  
NATURE COMMUNICATIONS, vol.10, 2019 (SCI-Expanded)
- XII. **A Noble-Metal-Free Heterogeneous Photosensitizer-Relay Catalyst Triad That Catalyzes Water Oxidation under Visible Light**  
Ghobadi T. G. U., YILDIZ E., BÜYÜKTEMİZ M., Akbari S. S., Topkaya D., İŞCİ Ü., DEDE Y., YAĞLIOĞLU H. G., KARADAŞ F.  
ANGEWANDTE CHEMIE-INTERNATIONAL EDITION, vol.57, no.52, pp.17173-17177, 2018 (SCI-Expanded)
- XIII. **Water Oxidation Electrocatalysis with a Cobalt-Borate-Based Hybrid System under Neutral Conditions**  
Turhan E. A., Nune S. V. K., ÜLKER E., Sahin U., DEDE Y., KARADAŞ F.  
CHEMISTRY-A EUROPEAN JOURNAL, vol.24, no.41, pp.10372-10382, 2018 (SCI-Expanded)
- XIV. **Tuning the Electronic Properties of Prussian Blue Analogues for Efficient Water Oxidation Electrocatalysis: Experimental and Computational Studies**  
Alsac E. P., ÜLKER E., Nune S. V. K., DEDE Y., KARADAŞ F.  
CHEMISTRY-A EUROPEAN JOURNAL, vol.24, no.19, pp.4856-4863, 2018 (SCI-Expanded)
- XV. **Different Quenching Effect of Intramolecular Rotation on the Singlet and Triplet Excited States of Bodipy**  
Lou Z., Hou Y., Chen K., Zhao J., Ji S., Zhong F., DEDE Y., Dick B.  
JOURNAL OF PHYSICAL CHEMISTRY C, vol.122, no.1, pp.185-193, 2018 (SCI-Expanded)
- XVI. **Nanostructured organic semiconductor films for molecular detection with surface-enhanced Raman spectroscopy**  
YILMAZ M., Babur E., Ozdemir M., Giesecking R. L., DEDE Y., TAMER U., Schatz G. C., Facchetti A., USTA H., DEMİREL G.  
NATURE MATERIALS, vol.16, no.9, pp.918-925, 2017 (SCI-Expanded)
- XVII. **H-bond stabilization of a tautomeric coumarin-pyrazole-pyridine triad generates a PET driven, reversible and reusable fluorescent chemosensor for anion detection**  
Alkis M., Pekyilmaz D., Yalcin E., AYDINER B., DEDE Y., SEFEROĞLU Z.  
DYES AND PIGMENTS, vol.141, pp.493-500, 2017 (SCI-Expanded)
- XVIII. **Synthesis and reactivity of a mononuclear non- haem cobalt(IV)-oxo complex**  
Wang B., Lee Y., Tcho W., Tussupbayev S., Kim S., Kim Y., Seo M. S., Cho K., DEDE Y., Keegan B. C., et al.  
NATURE COMMUNICATIONS, vol.8, 2017 (SCI-Expanded)
- XIX. **A fluorescent coumarin-thiophene hybrid as a ratiometric chemosensor for anions: Synthesis, photophysics, anion sensing and orbital interactions**  
Yanar U., Babur B., Pekyilmaz D., Yahaya I., AYDINER B., DEDE Y., SEFEROĞLU Z.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1108, pp.269-277, 2016 (SCI-Expanded)
- XX. **Morphological Versatility in the Self-Assembly of Val-Ala and Ala-Val Dipeptides**  
Erdogan H., Babur E., YILMAZ M., Candas E., GÖRDESEL YILDIZ M., DEDE Y., ÖREN E. E., Demirel G. B., Ozturk M. K., YAVUZ M. S., et al.  
LANGMUIR, vol.31, no.26, pp.7337-7345, 2015 (SCI-Expanded)
- XXI. **Intracellular Modulation of Excited-State Dynamics in a Chromophore Dyad: Differential Enhancement of Photocytotoxicity Targeting Cancer Cells**  
Kolemen S., Isik M., Kim G. M., Kim D., Geng H., Buyuktemiz M., Karatas T., Zhang X., DEDE Y., Yoon J., et al.

- ANGEWANDTE CHEMIE-INTERNATIONAL EDITION, vol.54, no.18, pp.5340-5344, 2015 (SCI-Expanded)
- XXII. **Synthesis and dye sensitized solar cell applications of Bodipy derivatives with bis-dimethylfluorenyl amine donor groups**  
Cakmak Y., Kolemen S., BÜYÜKTEMİZ M., DEDE Y., ERTEN ELA Ş.  
NEW JOURNAL OF CHEMISTRY, vol.39, no.5, pp.4086-4092, 2015 (SCI-Expanded)
- XXIII. **1,4,8,11,15,18,22,25-Alkylsulfanyl phthalocyanines: effect of macrocycle distortion on spectroscopic and packing properties**  
ZORLU Y., Kumru U., İŞÇİ Ü., Divrik B., Jeanneau E., Albrieux F., DEDE Y., AHSEN V., DUMOULIN F.  
CHEMICAL COMMUNICATIONS, vol.51, no.30, pp.6580-6583, 2015 (SCI-Expanded)
- XXIV. **Design and characterization of Bodipy derivatives for bulk heterojunction solar cells**  
Kolemen S., Cakmak Y., Ozdemir T., ERTEN ELA Ş., BÜYÜKTEMİZ M., DEDE Y., AKKAYA E. U.  
TETRAHEDRON, vol.70, no.36, pp.6229-6234, 2014 (SCI-Expanded)
- XXV. **Switching Off the Charge Transfer and Closing the S-1-T-1 ISC Channel in Excited States of Quinolizinium Derivatives: A Theoretical Study**  
Yalcin S., Thomas L., Tian M., SEFEROĞLU N., Ihmels H., DEDE Y.  
JOURNAL OF ORGANIC CHEMISTRY, vol.79, no.9, pp.3799-3808, 2014 (SCI-Expanded)
- XXVI. **Ion responsive near-IR BODIPY dyes: two isomers, two different signals**  
Ozdemir T., Kostereli Z., Guliyev R., Yalcin S., DEDE Y., AKKAYA E. U.  
RSC ADVANCES, vol.4, no.29, pp.14915-14918, 2014 (SCI-Expanded)
- XXVII. **Ni(II)-tetrahedral complexes: Characterization, antimicrobial properties, theoretical studies and a new family of charge-transfer transitions**  
SARI N., Sahin S. C., Ogutcu H., DEDE Y., Yalcin S., ALTUNDAŞ A., Doganay K.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.106, pp.60-67, 2013 (SCI-Expanded)
- XXVIII. **Luminescence of BODIPY and Dipyrrin: An MCSCF Comparison of Excited States**  
BÜYÜKTEMİZ M., Duman S., DEDE Y.  
JOURNAL OF PHYSICAL CHEMISTRY A, vol.117, no.7, pp.1665-1669, 2013 (SCI-Expanded)
- XXIX. **Heavy Atom Free Singlet Oxygen Generation: Doubly Substituted Configurations Dominate S-1 States of Bis-BODIPYs**  
Duman S., Cakmak Y., Kolemen S., AKKAYA E. U., DEDE Y.  
JOURNAL OF ORGANIC CHEMISTRY, vol.77, no.10, pp.4516-4527, 2012 (SCI-Expanded)
- XXX. **Reactions of 1S, 1D, and 3P carbon atoms with water. Oxygen abstraction and intermolecular formaldehyde generation mechanisms; An MCSCF study**  
ÖZKAN İ., DEDE Y.  
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, vol.112, no.4, pp.1165-1184, 2012 (SCI-Expanded)
- XXXI. **Intermolecular acetaldehyde and dimethoxymethane formation mechanisms via ethenol and methoxymethylene precursors in reactions of atomic carbon with methanol: a computational study**  
DEDE Y., ÖZKAN İ.  
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol.14, no.7, pp.2326-2332, 2012 (SCI-Expanded)
- XXXII. **Designing Excited States: Theory-Guided Access to Efficient Photosensitizers for Photodynamic Action**  
Cakmak Y., Kolemen S., Duman S., DEDE Y., Dolen Y., Kilic B., Kostereli Z., YILDIRIM L., Dogan A. L., Guc D., et al.  
ANGEWANDTE CHEMIE-INTERNATIONAL EDITION, vol.50, no.50, pp.11937-11941, 2011 (SCI-Expanded)
- XXXIII. **A Redox Non-Innocent Ligand Controls the Life Time of a Reactive Quartet Excited State - An MCSCF Study of [Ni(H)(OH)](+)**  
DEDE Y., Zhang X., Schlangen M., Schwarz H., Baik M.  
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, vol.131, no.35, pp.12634-12642, 2009 (SCI-Expanded)
- XXXIV. **DFT Studies on the Thermal Activation of Molecular Oxygen by Bare [Ni(H)(OH)](+)**  
Zhang X., Schlangen M., Baik M., DEDE Y., Schwarz H.  
HELVETICA CHIMICA ACTA, vol.92, no.1, pp.151-164, 2009 (SCI-Expanded)
- XXXV. **A panchromatic boradiazaindacene (BODIPY) sensitizer for dye-sensitized solar cells**

Erten-Ela S., YILMAZ M. S., Icli B., DEDE Y., Icli S., Akkaya E. U.  
ORGANIC LETTERS, vol.10, no.15, pp.3299-3302, 2008 (SCI-Expanded)

- XXXVI. **Determination of trace element levels in human scalp hair in occupationally exposed subjects by XRF**  
DEDE Y., Erten H., Zararsiz A., Efe N.  
Journal of Radioanalytical and Nuclear Chemistry, vol.247, no.2, pp.393-397, 2001 (SCI-Expanded)

### Refereed Congress / Symposium Publications in Proceedings

- I. **Two Short Stories on Radical Centers Involved in Non-radical Reactions: Dioxygen Activation by [(H)Ni(OH)] and Water Oxidation at Co-Oxo/Oxyl**  
DEDE Y.  
CPC XII, 12 - 13 October 2018
- II. **Quantum Chemical Analysis of O–O Bond Formation at Co(IV)-Oxo Center**  
DEDE Y., ŞAHİN U.  
CPC XII, 12 October 2018
- III. **On the Electronic Structure of Co(IV)-O Complexes**  
DEDE Y., Qandeel O.  
CPC XII, 12 - 13 October 2018
- IV. **Oxidative Methane Activation With Cationic Ligand-metal Complexes**  
DEDE Y., Ocak Y.  
CPC XII, 12 - 13 October 2018
- V. **Electronic Structure of BOPHY – When Does Adding Two Rings Not Make a Larger Ring?**  
Büyüktemiz M., Dede Y.  
CPC - XII, Karabük, Turkey, 12 - 13 October 2018
- VI. **Quantum Chemical Analysis of Intersystem Crossing in Organic Fluorophores**  
Yıldız D. B., Büyüktemiz M., Dede Y.  
CPC - XII, Karabük, Turkey, 12 - 13 October 2018
- VII. **QUANTUM CHEMICAL ANALYSIS OF O–O BOND FORMATION AT THE CO (IV) OXO CENTER**  
ŞAHİN U., yıldız o., DEDE Y.  
ECOSTBio, Berlin, 9 - 11 April 2018
- VIII. **THEORETICAL STUDY OF ACTIVATION OF DIOXYGEN BY [(H)Ni(OH)], NON-INNOCENCE OF HYDROXYL IS LOST BEFORE THE ACTIVATION STEP**  
DEDE Y.  
ECOSTBio Berlin, 9 - 11 April 2018
- IX. **[Ni(H)(OH)] ile Dioksijen Aktivasyonunun Kuramsal İncelenmesi**  
DEDE Y.  
Ulusal Kimya Kongresi, Turkey, 10 - 14 September 2017
- X. **Chromophore Excited States - Towards Predictive Theoretical Studies**  
DEDE Y.  
Second GTÜ Photodynamic Day, 16 May 2017
- XI. **Dioxygen Activation by HNiOH, An MCSCF Study**  
DEDE Y.  
COST 1305 ECOSTBio Lisbon, 30 - 31 March 2017
- XII. **Proton transfer without the Secondary Sphere Base**  
DEDE Y.  
COST Action CM1205 Carisma Lisbon, 6 - 08 March 2017
- XIII. **Proton transfer without the secondary sphere base computational study of an HPCD Mimic**  
DEDE Y.  
MOLMOD 2016, 13 - 15 November 2016
- XIV. **Theoretical Analysis of the BOPHY Fluorophore**

alkış m., DEDE Y.

MOLMOD 2016, 13 - 15 November 2016

**XV. Mimicking the Secondary Sphere of Homoprotocatechuate Dioxygenase HPCD Enzyme Active Site A Theoretical Study**

Büyüktemiz M., Dede Y.

COST ECOSTBio Meeting - Prague, Karabük, Turkey, 13 - 15 April 2016

**XVI. Secondary Sphere Histidine of Homoprotocatechuate Dioxygenase A Modified Model of the Enzymatic Core 21st 23rd 2016**

Büyüktemiz M., Dede Y.

COST Action CM1205 -CARISMA , Ljubljana, Karabük, Turkey, 21 - 23 March 2016

## Supported Projects

DEDE Y., Yıldız D. B., BÜYÜKTEMİZ M., Project Supported by Higher Education Institutions, BF2 Tabanlı Yeni Nesil Kromoforların Spektroskopik Özelliklerinin Kuantum Kimyasal İncelenmesi, 2021 - 2022

Dede Y., Çakmak Y., Kırbıyık Ç., TUBİTAK Project, Organik Güneş Hücrelerinde Uygulanmak Üzere Elektron Verici Moleküllerin Tasarım, Sentez ve Karakterizasyonu, 2018 - 2021

Dede Y., TUBİTAK Project, Katyonik ve Asidik Ligand - Metal Kompleksleri ile Oksidatif Metan Aktivasyonunun Kuramsal Tasarımı, 2017 - 2021

Dede Y., Demirel G., Usta H., TUBİTAK Project, Organik Yarı İletken Temelli 3-Boyutlu Mikro-/Nano-Yapılı Platformların Yüzey-Güçlendirilmiş Raman Spektroskopisinde (Sers) Kullanımları, 2018 - 2020

DEDE Y., Project Supported by Higher Education Institutions, Kuantum Kimyası Araştırma Laboratuvarının Altyapısının Güçlendirilmesi, 2016 - 2019

Dede Y., TÜBİTAK - AB COST Project, İndasen Tabanlı Yeni Floroforların Çok Referanslı Mcscf Metotlarla Kuantum Kimyasal Tasarımı, 2015 - 2017

Dede Y., TÜBİTAK - AB COST Project, Homoprotokatekolat Dioksijenaz Aktif Merkezinin Çok Referanslı MCSCF Kuantum Kimyasal Metotlarla İncelenmesi Biyoorganik Metal Kompleksleriyle Oksijen ve Katekol Türevlerine İlişkin Tepkime Mekanizmalarının Genelleştirilmesi, 2013 - 2015

DEDE Y., Project Supported by Higher Education Institutions, Çeşitli dipirin kromoforlarının elektronik yapılarının kuantum kimyasal incelenmesi, 2011 - 2013

Dede Y., TUBİTAK Project, Bor di-Pirometen Merkezli Floroforların (BODIPY) Uyarılmış Hallerinin Çok Referanslı (MCSCF) Metotlarla Kuantum Kimyasal İncelenmesi, 2011 - 2013