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Academic History

Professor: Gazi University, Ankara, Faculty of Science Department of Chemistry,
2022 – present

Associate Professor: Gazi University, Ankara, Faculty of Science Department of Chemistry,
2014 – 2022

Lecturer: Gazi University, Ankara, Faculty of Science Department of Chemistry,
2010 – 2014

Postdoctoral Research Associate: Indiana University – Bloomington, Department of Chemistry,

2007 – 2008. Research Group of Professor M. Baik.

2008 – 2009. Joint postdoctoral appointment in Research Groups of Professors M. Baik and S. Tait.

Ph.D.: Middle East Technical University, Ankara, Faculty of Arts and Sciences, Department of Chemistry (English) 2002 – 2007.

Thesis: Quantum Chemical Investigations of the Reactions of Atomic Carbon (C) with Water and Methanol

Supervisor: Prof. Dr. İlker Özkan

M.S.: Middle East Technical University, Ankara, Faculty of Arts and Sciences, Department of Chemistry (English) 1999 – 2002.

Thesis: Supramolecules for Constructing Nanoscale Devices

Supervisor: Prof. Dr. Engin Umut Akkaya

B.S.: Bilkent University, Ankara, Faculty of Science Department of Chemistry (English)
1995 – 1999. (Full undergraduate scholarship)

Awards and Degrees

8) Turkish Academy of Sciences, Young Scientist Award (GEBİP), **2015**.

7) Turkish Science Academy Foundation, Young Scientist Award (BAGEP), **2015**.

6) ODTÜ Mustafa N. Parlar Foundation, Young Scientist Award, **2014**.

5) TÜBİTAK Postdoctoral Scholarship, **2008**.

4) Bilkent University Undergraduate Scholarship, **1995 – 1999**.

3) TÜBİTAK University Entrance Examination Scholarship, **1995**.

2) National University Entrance Examination, (8th in ranking in the nationwide exam among ~1,500,000 students), **1995**.

1) High School: Milli Piyango Anatolian High School (English), Ankara (ranking the 2nd in the graduate class of **1995**)

Projects supervised and funds raised (total ~USD 495000 = ~EUR 400 000)

- 6) GÜ-BAP, Project leader, **05/2021 – 06/2022**. Budget: ~10 000 USD
 7) TÜBİTAK – 1001, 114Z337, Project leader, **10/2017 – 10/2020**. ~100 000 USD
 6) GÜ-BAP, Project leader, **05/2016 – 06/2016**. Budget: ~100 000 USD
 5) TÜBİTAK/COST (ECOSTBio) – 1001, 114Z790, Project leader, **2015 - 2017**. ~80 000 USD
 4) TÜBİTAK – 1001, 114Z980, co-supervisor, **2015 - 2018**. ~120 000 USD
 3) TÜBİTAK/COST (CARISMA) 212To47, Project leader, **04/2013 - 10/2015**. ~50 000 USD
 2) TÜBİTAK Early career project, 110T647, Project leader, **04/2011 – 04/2013**. ~40 000 USD
 1) GÜ-BAP, Project leader, **05/2011 – 05/2013**. Budget: ~5 000 USD

TÜBİTAK: Scientific and Technological Research Council of Turkey

GÜ-BAP: Gazi University, Scientific Research Projects Office

Details of Selected Projects Supervised by Dr. Dede

Code	Type	Start	Duration (months)	Status	Budget (share of the host institution)
114Z337	TÜBİTAK 1001	10/2017	36	Completed	365,880 TL (91,680 TL)
114Z790	TÜBİTAK 1001/COST (CM 1305)	05/2015	24	Completed	268,805 TL (69, 088 TL)
212To47	TÜBİTAK 1001/COST (CM 1205)	04/2013	30	Completed	176,750 TL (13,000 TL)
110T647	TÜBİTAK 3501	04/2011	24	Completed	103,330 TL (7,575 TL)

Details of Projects Contributed by Dr. Dede

Code	Scope	Type	Role	Start	End
118Z392	Quantum Chemical Design of Dyes for Applications in Solar Cells	TÜBİTAK 3501	Researcher/Expert	12/2018	12/2021
117F468	Quantum Chemical Analysis of Organic Surface Enhanced Raman Spectroscopy (SERS)	TÜBİTAK 1001	Consultant	05/2018	05/2021
114Z980	Quantum Chemical Design of Thiophene based Receptors	TÜBİTAK 1001	Researcher/Expert	06/2015	09/2017

Research Interests

Theoretical/Computational Chemistry.

Mechanistic understanding of small molecule (O_2 , CH_4 , CO_2 , H_2O) activation reactions catalyzed by transition metal complexes. Manifestations of spin states.

Excited states of organic chromophores.

Application of multi-reference *ab initio* methods such as CASSCF and CAS-MP2. Molecular excited states, non-adiabatic reaction mechanisms, curve crossings, near degeneracies.

Selected Representative Publications

	Title	Journal	Volume/Page/Year
1	Heavy Atom Free Singlet Oxygen Generation: Doubly Substituted Configurations Dominate S-1 States of Bis-BODIPYs (FEATURED ARTICLE)	THE JOURNAL OF ORGANIC CHEMISTRY	77 4516-4527 2012
2	Luminescence of BODIPY and Dipyrin: An MCSCF Comparison of Excited States	JOURNAL OF PHYSICAL CHEMISTRY A	117 1665-1668 2013
3	Intermolecular acetaldehyde and dimethoxymethane formation mechanisms via ethenol and methoxymethylene precursors in reactions of atomic carbon with methanol: a computational study	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	14 2326-2332 2012
4	When Does Fusing Two Rings Not Yield a Larger Ring? The Curious Case of BOPHY. The Journal of Organic Chemistry,	THE JOURNAL OF ORGANIC CHEMISTRY	86 4547-4556 2021
5	A Robust, Precious-Metal-Free Dye-Sensitized Photoanode for Water Oxidation: A Nanosecond-Long Excited State Lifetime through a Prussian Blue Analogue (COVER FEATURE)	ANGEWANDTE CHEMIE-INTERNATIONAL EDITION	10.1002/ange.201914743 2020
6	Water Oxidation Electrocatalysis with a Cobalt-Borate-Based Hybrid System under Neutral Conditions (COVER FEATURE, HOT PAPER)	CHEMISTRY A EUROPEAN JOURNAL	24 10372-10382 2018
7	A Redox Non-Innocent Ligand Controls the Life Time of a Reactive Quartet Excited State - An MCSCF Study of $[Ni(H)(OH)](+)$	JOURNAL OF THE AMERICAN CHEMICAL SOCIETY	131 12634-12642 2009
8	Designing Excited States: Theory-Guided Access to Efficient Photosensitizers for Photodynamic Action	ANGEWANDTE CHEMIE-INTERNATIONAL EDITION	50 11937-11941 2011

Selected Publications from Collaborations

8	<i>Angewandte Chemie International Edition</i> , 10.1002/ange.201914743, (2020). Cover feature.
7	<i>Nature Communications</i> , 10, 276 (2019).
6	<i>Angewandte Chemie International Edition</i> , 57, 17173, (2018).
5	<i>Nature Materials</i> , 16, 918 (2017).
4	<i>Nature Communications</i> , 8, 14839 (2017).
3	<i>Chemical Communications</i> , 51, 6580 (2015).
2	<i>Angewandte Chemie International Edition</i> , 54, 5340 (2015). Cover feature.
1	<i>Angewandte Chemie International Edition</i> , 50, 11937 (2011).

Selected Invited Talks

- 9)** ECOSTBio Meeting, Berlin, Germany, **2018**.
- 8)** Second GTU Photodynamic Day, Gebze, Turkey, **2015**.
- 7)** RSC Symposium - Catalysis and Sensing for Health, Ankara, Turkey, **2015**.
- 6)** Dalian University of Technology, Dalian, Peoples Republic of China, **2015**.
- 5)** International Conference on Porphyrins and Phthalocyanines (ICPP-8) - İstanbul, **2014**.
- 4)** National Computational Chemistry Workshop, Van, Turkey, **2014**.
- 3)** X Girona Seminar on Theoretical and Computational Chemistry for the Modeling of Biochemical Systems - From Theory to Applications, Girona, Spain, **2012**.
- 2)** Indiana University - Bloomington, USA, **2012**.
- 1)** Imperial College - London, UK, **2011**.

Thesis Supervised

- 11)** Muhammed **Büyüktemiz**, Gazi University, Ph.D., continuing.
- 10)** Dilara Berna **Yıldız**, Gazi University, Ph.D., continuing.
- 9)** Osama **Qandeel**, Gazi University, M.S., 2022.
- 8)** Dilara Berna **Yıldız**, Gazi University, M.S., 2020.
- 7)** Gözde **Papır**, Gazi University, M.S., continuing.
- 6)** Yıldız **Ocak**, Gazi University, M.S., **2020**.
- 5)** Ufuk **Şahin**, Gazi University, M.S., **2020**.
- 4)** Muhammed **Büyüktemiz**, Gazi University, M.S., **2020**.
- 3)** Soydan **Yalçın**, Gazi University, M.S., **2015**.
- 2)** Gökçe **Alıcı**, Gazi University, M.S., **2012**.
- 1)** Selin **Duman**, Gazi University, M.S., **2012**.

Industrial and Commercial Experience

Turkish Standards Institution Product Certification Center, Chemist, Certification of Insulation Products, Ankara, TURKEY (2006 - 2009)

Teaching*

Introduction to Quantum Chemistry, Faculty of Science, Department of Chemistry
Mathematics for Chemists, Faculty of Science, Department of Chemistry
Introduction to Computational Chemistry, Faculty of Science, Department of Chemistry

Theoretical Chemistry, Graduate School of Science, Department of Chemistry

General Chemistry I, Faculty of Engineering, Department of Chemical Engineering
General Chemistry II, Faculty of Engineering, Department of Chemical Engineering

**A full list of all the courses are available upon request.*

Language

English; has been educated in English since secondary school (age 11). Most of the courses including mathematics and science were taught in English after grade 5. College, M.S. and Ph.D. are completed in institutions (Bilkent Univ. and METU) where all the education is in English.

Brief Research Statement

I've studied the reaction mechanisms of reactive intermediates found in the inter-stellar medium in my PhD. I've suggested novel paths for organic molecule formation in collision of carbon atoms with frozen matrices thereby explaining the formation of all of the observed products. The results have implications about the origin of organic matter in space. High level ab-initio electron correlation techniques were used for those analyses. As representative works please see publications 6 (*PCCP*, **2012**) and 8 (*IJQC*, **2012**).

As a postdoctoral researcher I've investigated non-adiabatic reactions of a small cationic complex that can activate (similar to methanotrophic bacteria) both methane and dioxygen using post-SCF techniques. As a representative work please see publication 3 (*JACS*, **2009**).

In my independent position as an Asst. and Assoc. Prof. at Gazi Univ. Ankara, Turkey, I've worked on various electronic states of organic molecules, their interaction with light and non-adiabatic reactions as well as establishing an understanding for their light induced device performances. We managed to identify some unique phenomena in explaining inter system crossing. Along with standard computational techniques we've mainly employed the Multi Configurational Self Consistent Field (MCSCF) technique. As representative works please see publications 7 (*JOC*, **2012**), 9 (*JPC-A*, **2013**) and 13 (*JOC* (**2014**)).

We're also studying the reactivity patterns of various small molecules under catalytic conditions as alternatives to global problem of energy. As representative works please see publications 23 (*CEJ*, **2018**), 24 (*CEJ*, **2018**), 25 (*ACIE*, **2018**), 27 (*ACIE*, **2020**), and 32 (*IC*, **2022**).

In the near future my recent work on excited states and small molecule activation reactions will continue. My experience in cases where, i) a multitude of electronic states coexist, and ii) reaction mechanisms of small molecules, will be combined to study photochemical reactions.

My research especially MCSCF computations are highly technical and difficult to deal with. On the other hand we are always making strong emphasis to the conceptual side of those demanding calculation results. Our predictions made purely on excited state calculations are already shown to be correct with further experiments or simple relations among excited state wave functions can guide further experiments.

We have worked in close contact with experimentalists and continue to contribute to the literature that way. This approach will keep being at the heart of my research in the near future. My experience in high level ab-initio electron correlation techniques will allow me to model almost the most complex electronic structure problems.

In summary my goal is performing truly-predictive theoretical studies using detailed electronic structure arguments and working in close collaborations with experimentalists.

An expanded research statement is available upon request.

Full List of Publications

	Please refer to my Google Scholar page for the most up to date list of publications
33	Tok, M.; Say, B.; Dölek, G.; Tatar, B.; Özgür, D. Ö.; Kurukavak, Ç. K.; Kuş, M.; Dede, Y.; Çakmak, Y., Substitution effects in distyryl BODIPYs for near infrared organic photovoltaics. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 429, 113933 (2022).
32	Ahmad, A. A.; Ulusoy Ghobadi, T. G.; Buyuktemiz, M.; Ozbay, E.; Dede, Y.; Karadas, F., Light-Driven Water Oxidation with Ligand-Engineered Prussian Blue Analogues. <i>Inorganic Chemistry</i> , 61 (9), 3931-3941 (2022).
31	Ghobadi, T. G. U.; Ghobadi, A.; Demirtas, M.; Buyuktemiz, M.; Ozvural, K. N.; Yildiz, E. A.; Erdem, E.; Yaglioglu, H. G.; Durgun, E.; Dede, Y.; Ozbay, E.; Karadas, F., Building an Iron Chromophore Incorporating Prussian Blue Analogue for Photoelectrochemical Water Oxidation. <i>Chemistry – A European Journal</i> , 27 (35), 8966-8976 (2021).
30	Buyuktemiz, M.; Kılıç, M.; Che, Y.; Zhao, J.; Dede, Y. When Does Fusing Two Rings Not Yield a Larger Ring? The Curious Case of BOPHY. <i>The Journal of Organic Chemistry</i> , 86, 6, 4547, (2021).
29	Dede, Y.; Yalcin, S.; Buyuktemiz, M., Excited state structures projected onto two dimensions: correlations with luminescent behavior. <i>Journal of Mathematical Chemistry</i> , (10), 2254-2272, (2020).
28	Sahibbeyli, V.; Yildiz, D. B.; Papir, G.; Dede, Y.; Demirel, G., The Role of Molecular Structure of Phenylalanine Peptides on the Formation of Vertically Aligned Ordered Bionanostructures: Implications for Sensing Application. <i>ACS Applied Nano Materials</i> , 3 (5), 4305-4313 (2020).
27	Ulusoy Ghobadi, T.G., Ghobadi, A., Buyuktemiz, M., Yildiz, E.A., Berna Yildiz, D., Yaglioglu, H.G., Dede, Y., Ozbay, E., and Karadas, F. A Robust, Precious-Metal-Free Dye-Sensitized Photoanode for Water Oxidation: A Nanosecond-Long Excited State Lifetime through a Prussian Blue Analogue. <i>Angew. Chem. Int. Ed.</i> 59, 10, 4082 (2020).
26	Cezan, S. D.; Nalbant, A. A.; Buyuktemiz, M.; Dede, Y.; Baytekin, H. T.; Baytekin, B. Control of Triboelectric Charges on Common Polymers by Photoexcitation of Organic Dyes. <i>Nature Communications</i> , 10, 276 (2019).
25	Ulusoy Ghobadi, G.; Akhuseyin Yildiz, E.; Buyuktemiz, M.; Akbari, S. S.; Topkaya, D.; İsci, Ü.; Dede, Y.; Yaglioglu, H. G.; Karadas, F., A Noble-Metal-Free Heterogeneous Photosensitizer-Relay-Catalyst Triad Catalyzes Water Oxidation under Visible Light, <i>Angew. Chem. Int. Ed.</i> 57, 17173 (2018).
24	Turhan, E. A., Nune, S. V. K., Ulker, E., Sahin, U., Dede, Y. & Karadas, F. Water Oxidation Electrocatalysis with a Cobalt-Borate-Based Hybrid System under Neutral Conditions. <i>Chemistry – A European Journal</i> , 24 (41), 10372-10382 (2018).
23	Pınar, A. E., Emine, Ü., Kumar, N. S. V., Yavuz, D. & Ferdi, K. Tuning the Electronic Properties of Prussian Blue Analogues for Efficient Water Oxidation Electrocatalysis: Experimental and Computational Studies. <i>Chemistry – A European Journal</i> , 24, 4856-63 (2018).
22	Lou, Z., Hou, Y., Chen, K., Zhao, J., Ji, S., Zhong, F., Dede, Y. & Dick, B. Different Quenching Effect of Intramolecular Rotation on the Singlet and Triplet Excited States of Bodipy. <i>The Journal of Physical Chemistry C</i> , 122, 185-93 (2018).
21	Yilmaz, M., Babur, E., Ozdemir, M., Giesecking, R. L., Dede, Y., Tamer, U., Schatz, G. C., Facchetti, A., Usta, H. & Demirel, G. Nanostructured organic semiconductor films for molecular detection with surface-enhanced Raman spectroscopy. <i>Nature Materials</i> , 16, 918-24 (2017).
20	Wang, B., Lee, Y.-M., Tcho, W.-Y., Tussupbayev, S., Kim, S.-T., Kim, Y., Seo, M. S., Cho, K.-B., Dede, Y., Keegan, B. C., Ogura, T., Kim, S. H., Ohta, T., Baik, M.-H., Ray, K., Shearer, J. & Nam, W. Synthesis and reactivity of a mononuclear non-haem cobalt(IV)-oxo complex. <i>Nature Communications</i> , 8, 14839 (2017).
19	Alkış, M., Pekyılmaz, D., Yalçın, E., Aydın, B., Dede, Y. & Seferoğlu, Z. H-bond stabilization of a tautomeric coumarin-pyrazole-pyridine triad generates a PET driven, reversible and reusable fluorescent chemosensor for anion detection. <i>Dyes and Pigments</i> , 141, 493-500 (2017).
18	Yanar, U., Babur, B., Pekyılmaz, D., Yahaya, I., Aydın, B., Dede, Y. & Seferoğlu, Z. A fluorescent coumarin-thiophene hybrid as a ratiometric chemosensor for anions: Synthesis, photophysics, anion sensing and orbital interactions. <i>Journal of Molecular Structure</i> , 1108, 269-77 (2016).
17	Zorlu, Y., Kumru, U., İsci, U., Divrik, B., Jeanneau, E., Albrieux, F., Dede, Y., Ahsen, V. & Dumoulin, F. 1,4,8,11,15,18,22,25-Alkylsulfanyl phthalocyanines: effect of macrocycle distortion on spectroscopic and packing properties. <i>Chemical Communications</i> , 51, 6580-3 (2015).
16	Kolemen, S., Işık, M., Kim, G. M., Kim, D., Geng, H., Buyuktemiz, M., Karatas, T., Zhang, X.-F., Dede, Y., Yoon, J. & Akkaya, E. U. Intracellular Modulation of Excited-State Dynamics in a Chromophore Dyad: Differential Enhancement of Photocytotoxicity Targeting Cancer Cells. <i>Angewandte Chemie International Edition</i> , 54, 5340-4 (2015).

15	Erdogan, H., Babur, E., Yilmaz, M., Candas, E., Gordesel, M., Dede, Y., Oren, E. E., Demirel, G. B., Ozturk, M. K., Yavuz, M. S. & Demirel, G. Morphological Versatility in the Self-Assembly of Val-Ala and Ala-Val Dipeptides. <i>Langmuir</i> , 31, 7337-45 (2015).
14	Cakmak, Y., Kolemen, S., Buyuktemiz, M., Dede, Y. & Erten-Ela, S. Synthesis and dye sensitized solar cell applications of Bodipy derivatives with bis-dimethylfluorenyl amine donor groups. <i>New Journal of Chemistry</i> , 39, 4086-92 (2015).
13	Yalcin, S., Thomas, L., Tian, M. Q., Seferoglu, N., Ihmels, H. & Dede, Y. Switching Off the Charge Transfer and Closing the S-1-T-1 ISC Channel in Excited States of Quinolizinium Derivatives: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 79, 3799-808 (2014).
12	Ozdemir, T., Kostereli, Z., Guliyev, R., Yalcin, S., Dede, Y. & Akkaya, E. U. Ion responsive near-IR BODIPY dyes: two isomers, two different signals. <i>RSC Advances</i> , 4, 14915-8 (2014).
11	Kolemen, S., Cakmak, Y., Ozdemir, T., Erten-Ela, S., Buyuktemiz, M., Dede, Y. & Akkaya, E. U. Design and characterization of Bodipy derivatives for bulk heterojunction solar cells. <i>Tetrahedron</i> , 70, 6229-34 (2014).
10	Sari, N., Sahin, S. C., Ogutcu, H., Dede, Y., Yalcin, S., Altundas, A. & Doganay, K. Ni(II)-tetrahedral complexes: Characterization, antimicrobial properties, theoretical studies and a new family of charge-transfer transitions. <i>Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy</i> , 106, 60-7 (2013).
9	Buyuktemiz, M., Duman, S. & Dede, Y. Luminescence of BODIPY and Dipyrin: An MCSCF Comparison of Excited States. <i>The Journal of Physical Chemistry A</i> , 117, 1665-9 (2013).
8	Ozkan, I. & Dede, Y. Reactions of 1S, 1D, and 3P carbon atoms with water. Oxygen abstraction and intermolecular formaldehyde generation mechanisms; An MCSCF study. <i>International Journal of Quantum Chemistry</i> , 112, 1165-84 (2012).
7	Duman, S., Cakmak, Y., Kolemen, S., Akkaya, E. U. & Dede, Y. Heavy Atom Free Singlet Oxygen Generation: Doubly Substituted Configurations Dominate S1 States of Bis-BODIPYs. <i>The Journal of Organic Chemistry</i> , 77, 4516-27 (2012).
6	Dede, Y. & Ozkan, I. Intermolecular acetaldehyde and dimethoxymethane formation mechanisms via ethenol and methoxymethylene precursors in reactions of atomic carbon with methanol: a computational study. <i>Physical Chemistry Chemical Physics</i> , 14, 2326-32 (2012).
5	Cakmak, Y., Kolemen, S., Duman, S., Dede, Y., Dolen, Y., Kilic, B., Kostereli, Z., Yildirim, L. T., Dogan, A. L., Guc, D. & Akkaya, E. U. Designing Excited States: Theory-Guided Access to Efficient Photosensitizers for Photodynamic Action. <i>Angewandte Chemie International Edition</i> , 50, 11937-41 (2011).
4	Zhang, X., Schlangen, M., Baik, M. H., Dede, Y. & Schwarz, H. DFT Studies on the Thermal Activation of Molecular Oxygen by Bare [Ni (H)(OH)]+. <i>Helvetica Chimica Acta</i> , 92, 151-64 (2009).
3	Dede, Y., Zhang, X., Schlangen, M., Schwarz, H. & Baik, M.-H. A Redox Non-Innocent Ligand Controls the Life Time of a Reactive Quartet Excited State - An MCSCF Study of [Ni(H)(OH)]+. <i>Journal of the American Chemical Society</i> , 131, 12634-42 (2009).
2	Erten-Ela, S., Yilmaz, M. D., Icli, B., Dede, Y., Icli, S. & Akkaya, E. U. A panchromatic boradiazaindacene (BODIPY) sensitizer for dye-sensitized solar cells. <i>Organic Letters</i> , 10, 3299-302 (2008).
1	Dede, Y., Erten, H. N., Zararsiz, A. & Efe, N. Determination of trace element levels in human scalp hair in occupationally exposed subjects by XRF. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 247, 393-7 (2001).

References^a

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^aMore references are available upon request