

**SAMER GOZEM, PH.D**  
**CURRICULUM VITAE**

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## Education

**Ph.D. (2008 – 2013)** in Photochemical Sciences, Bowling Green State University (BGSU).  
Thesis: “*Understanding the Relationship Between Thermal and Photochemical Isomerization in Visual Receptors.*” [Link to Dissertation](#).

Advisor: Prof. Massimo Olivucci

**Cert. (2010 – 2013)** Graduate certificate in Bioinformatics and Proteomics/Genomics, Bowling Green State University (BGSU) and University of Toledo (UToledo).

**B.Sc. (2005 – 2008)** *Summa Cum-Laude* in Chemistry with a minor in Business Administration, American University of Beirut (AUB).

## Professional Experience

**2017 – present** Assistant Professor of Chemistry. Georgia State University.

**2014 – 2017** Postdoctoral Research. University of Southern California.

Advisor: Prof. Anna I. Krylov

## Awards and Honors

**2014** Burg Foundation Postdoctoral Teaching Award, Department of Chemistry, USC.

**2014** Postdoctoral Scholars Training & Travel Grant, Office of Postdoctoral Affairs, USC.

**2014** Distinguished Dissertation Award, Graduate College, BGSU.

**2013** Outstanding Dissertation Award, Department of Chemistry, BGSU.

**2013** Katzner Graduate Student Research and Professional Development, Graduate College, BGSU.

**2010** Outstanding Teaching Assistant award, Department of Chemistry, BGSU.

**2008** *Summa Cum-Laude* honor with B.Sc., Faculty of Arts and Sciences, AUB

**2005 - 2008** Dean’s Honor List, Faculty of Arts and Sciences, AUB.

## Publications

### Book Chapter

*Computational Photochemistry and Photobiology.*

El-Khoury PZ, Schapiro I, Huntress M, Melaccio F, [Gozem S](#), Frutos LM, Olivucci M

In ***CRC Handbook of Organic Photochemistry and Photobiology***; Griesbeck A, Oelgemöller M, and Ghetti F, Ed.; CRC press: USA, **2012**. [Link to Chapter](#).

## Journal Articles

27. *Vacuum Ultraviolet Photoionization Cross Section of the Hydroxyl Radical.*  
Dodson LG; Savee JD; [Gozem S](#); Shen L; Krylov AI; Taatjes CA; Osborn DL; Okumura M.  
**J. Chem. Phys.** 148, 184302. 2018. [Link to Article](#).
26. *Theory and Simulation of the Ultrafast Double-Bond Isomerization of Biological Chromophores.*  
[Gozem S](#); Luk HL; Schapiro I; Olivucci M.  
**Chem. Rev.** 117, 13502–13565. 2017. [Link to Article](#).
25. *Supramolecular Sensors for Opiates and Their Metabolites.*  
Shcherbakova E, Zhang B, [Gozem S](#), Minami T, Zavalij P, Pushina M, Isaacs L, Anzenbacher P  
**J. Am. Chem. Soc.** 139, 14954–14960. 2017. [Link to Article](#).  
- Featured as a Spotlight and is on the front cover of JACS. [Link to Spotlight](#).
24. *Photoelectron Spectroscopy Study of Quinonimides.*  
Hossain E, Deng SM, [Gozem S](#), Krylov AI, Wang XB, Wenthold PG  
**J. Am. Chem. Soc.** 139, 11138–11148. 2017. [Link to Article](#).
23. *Electronic Spectra of Tris(2,2'-bipyridine)-M(II) Complex Ions in Vacuo (M = Fe and Os).*  
Xu S, Smith J, [Gozem S](#), Krylov AI, Weber JM  
**Inorg. Chem.** 56, 7029–7037. 2017. [Link to Article](#).
22. *Fluorescence-Based Assay for Carbonic Anhydrase Inhibitors.*  
Koutnik P, Shcherbakova EG, Caglayan MG, [Gozem S](#), Minami T, Anzenbacher P  
**Chem.** 2, 271–282. 2017. [Link to Article](#).
21. *A Study of Interstellar Aldehydes and Enols as Tracers of a Cosmic Ray-Driven Nonequilibrium Synthesis of Complex Organic Molecules.*  
Abplanalp MJ, [Gozem S](#), Krylov AI, Shingledecker CN, Herbst E, Kaiser RI  
**Proc. Natl. Acad. Sci. U.S.A.** 113, 7727–7732. 2016. [Link to Article](#).
20. *Probing the Photodynamics of Rhodopsins with Reduced Retinal Chromophores.*  
Manathunga M, Yang X, Luk HL, [Gozem S](#), Frutos LM, Valentini A, Ferré N, Olivucci M  
**J. Chem. Theory Comput.** 12, 839–850. 2016. [Link to Article](#).
19. *Ligand Influence on the Electronic Spectra of Monocationic Copper–Bipyridine Complexes.*  
Xu S, [Gozem S](#), Krylov AI, Christopher CR, Weber JM  
**Phys. Chem. Chem. Phys.** 17, 31938–31946. 2015. [Link to Article](#).
18. *Photoelectron Wave Function in Photoionization: Plane wave or Coulomb wave?*  
[Gozem S](#), Gunina AO, Ichino T, Osborn DL, Stanton JF, Krylov AI  
**J. Phys. Chem. Lett.** 6, 4532–4540. 2015. [Link to Article](#). [Link to ACS Liveslides](#).
17. *Molecular Bases for the Selection of the Chromophore of Animal Rhodopsins.*  
Luk HL, Melaccio F, Rinaldi S, [Gozem S](#), Olivucci M  
**Proc. Natl. Acad. Sci. U.S.A.** 112, 15297–15302. 2015. [Link to Article](#).
16. *Assessment of Approximate Coupled-Cluster and Algebraic-Diagrammatic-Construction Methods for Ground- and Excited-State Reaction Paths and the Conical-Intersection Seam of a Retinal-Chromophore Model.*  
Tuna D, Lefrancois D, Wolański Ł, [Gozem S](#), Schapiro I, Andruniów T, Dreuw A, Olivucci M  
**J. Chem. Theory Comput.** 11, 5758–5781. 2015. [Link to Article](#).

15. *Quantum Monte Carlo Treatment of the Charge Transfer and Diradical Electronic Character in a Retinal Chromophore Minimal Model.*  
Zen A, Coccia E, [Gozem S](#), Olivucci M, Guidoni L  
**J. Chem. Theory Comput.** 11, 992–1005. 2015. [Link to Article](#).
14. *A Conical Intersection Controls the Deactivation of the Bacterial Luciferase Fluorophore.*  
[Gozem S](#), Mirzakulova E, Schapiro I, Melaccio F, Glusac KD, Olivucci M  
**Angew. Chem. Int. Ed.** 53, 9870–9875. 2014. [Link to Article](#).
13. *Shape of Multireference, Equation-of-Motion Coupled-Cluster, and Density Functional Theory Potential Energy Surfaces at a Conical Intersection.*  
[Gozem S](#), Melaccio F, Valentini A, Filatov M, Huix-Rotllant M, Ferré N, Frutos LM, Angeli C, Krylov AI, Granovsky AA, Lindh R, Olivucci M  
**J. Chem. Theory Comput.** 10, 3074–3084. 2014. [Link to Article](#).
12. *Learning from Photobiology how to Design Molecular Devices Using a Computer.*  
[Gozem S](#), Melaccio F, Luk HL, Rinaldi S, Olivucci M  
**Chem. Soc. Rev.** 43, 4019-4036. 2014. [Link to Article](#)  
- Hot Chem. Soc. Rev. article for July 2014.
11. *Comparison of the Isomerization Mechanisms of Human Melanopsin and Invertebrate and Vertebrate Rhodopsins.*  
Rinaldi S, Melaccio F, [Gozem S](#), Fanelli F, Olivucci M  
**Proc. Natl. Acad. Sci. U.S.A.** 111, 1714–1719. 2014. [Link to Article](#).
10. *Probing Vibrationally Mediated Ultrafast Excited-State Reaction Dynamics with Multireference (CASPT2) Trajectories.*  
El-Khoury PZ, Joseph S, Schapiro I, [Gozem S](#), Olivucci M, Tarnovsky AN  
**J. Phys. Chem. A.** 117, 11271–11275. 2013. [Link to Article](#).
9. *Mapping the Excited State Potential Energy Surface of a Retinal Chromophore Model with Multireference and Equation-of-Motion Coupled-Cluster Methods.*  
[Gozem S](#), Melaccio F, Lindh R, Krylov AI, Granovsky AA, Angeli C, Olivucci M  
**J. Chem. Theory Comput.** 9, 4495–4506. 2013. [Link to Article](#).
8. *Towards an Understanding of the Retinal Chromophore in Rhodopsin Mimics.*  
Huntress MM, [Gozem S](#), Malley K, Jailaubekov A, Vasileiou C, Vengris M, Geiger J, Borhan B, Schapiro I, Larsen D, Olivucci M  
**J. Phys. Chem. B.** 117, 10053–10070. 2013. [Link to Article](#).
7. *Assessment of Density Functional Theory for Describing the Correlation Effects on the Ground and Excited State Potential Energy Surfaces of a Retinal Chromophore Model.*  
Huix-Rotllant M, Filatov M, [Gozem S](#), Schapiro I, Olivucci M, Ferré N  
**J. Chem. Theory Comput.** 9, 3917–3932. 2013. [Link to Article](#).
6. *Combined Self-Consistent-Field and Spin-Flip Tamm-Dancoff Density Functional Approach to Potential Energy Surfaces for Photochemistry.*  
Xu X, [Gozem S](#), Olivucci M, Truhlar D  
**J. Phys. Chem. Lett.** 4, 253–258. 2013. [Link to Article](#).
5. *Conical Intersection and Potential Energy Surface Features of a Model Retinal Chromophore: Comparison of EOM-CC and Multireference Methods.*  
[Gozem S](#), Krylov AI, Olivucci M  
**J. Chem. Theory Comput.** 9, 284–292. 2013. [Link to Article](#).

4. *Dynamic Electron Correlation Effects on the Ground State Potential Energy Surface of a Retinal Chromophore Model.*  
Gozem S., Huntress MM, Schapiro I, Lindh R, Granovsky AA, Angeli C, Olivucci M  
**J. Chem. Theory Comput.** 8, 4069–4080. 2012. [Link to Article.](#)
3. *The Molecular Mechanism of Thermal Noise in Rod Photoreceptors.*  
Gozem S., Schapiro I, Ferré N, Olivucci M  
**Science.** 137, 1225–1228. 2012. [Link to Article.](#)  
 - Editor's Choice. Vinson, V. Responding to Light and Heat. *Science Signaling.* 2012. [Link.](#)
2. *Origin of Fluorescence in 11-cis Locked Bovine Rhodopsin.*  
 Laricheva EN, Gozem S., Rinaldi S, Melaccio F, Valentini A, Olivucci M  
**J. Chem. Theory Comput.** 8, 2559–2563. 2012. [Link to Article.](#)
1. *Calculations on the Kinetics, Thermodynamics, and Selectivity of Methyl Radical Addition to Olefins Coordinated to  $d^8$  and  $d^0$  Transition-Metal Fragments: Two Distinct and Opposite anti-Evans–Polanyi Effects with Potential Practical Implications*  
 Hasanayn F, Gozem S.  
**Organometallics.** 27, 5426–5429. 2008. [Link to Article.](#)

## Conferences and Workshops

### Conference Presentations

9. *Calculating Photoionization and Photodetachment Spectra from Correlated Wave Functions.*  
Gozem S., Krylov AI  
**ACS National Meeting**, Philadelphia, PA. 2016.
8. *Photoelectron Spectra and Photoelectron Angular Distributions From Correlated Dyson Orbitals.*  
Gozem S., Krylov AI  
**TSRC: Advanced Particle Imaging Techniques: 1986-2016 and beyond**, Telluride, CO. 2016.  
 - “Hot topic” talk
7. *Photoionization and Photodetachment Spectra From Equation-of-Motion Coupled-Cluster Dyson Orbitals.*  
Gozem S., Gunina A, Krylov AI  
**ACS National Meeting**, San Diego, CA. 2016.
6. *Photoelectron Wave Function in Photoionization: Plane Wave or Coulomb Wave?*  
Gozem S., Osborn DL, Stanton JF, Krylov AI  
**ACS National Meeting**, San Diego, CA. 2016.
5. *Photoionization and Photodetachment Spectra From Equation-of-Motion Coupled-Cluster Dyson Orbitals.*  
Gozem S., Krylov AI  
**Sanibel Symposium**, St. Simons Island, GA. 2016.
4. *Calculations of Photoionization and Photodetachment Cross Sections using Correlated Dyson Orbitals and Simple Model Wavefunctions of the Ejected Electrons.*  
Gozem S., Krylov AI  
**Molecular & Ionic Clusters Gordon Research Conference**, Ventura, CA. 2016.  
 - “Late-Breaking Topic” presentation

3. *Photoelectron Spectra and Photoelectron Angular Distributions From Ab Initio Electronic Structure Methods.*  
Gozem S., Krylov AI  
**ACS National Meeting**, Denver, CO. **2015.**
2. *Molecular Mechanism of Thermal Noise in Rod Photoreceptors: When the Ultraslow Competes with the Ultrafast.*  
Gozem S., Schapiro I, Ferré N, Olivucci M  
**ACS National Meeting**, Dallas, TX. **2014.**
1. *The Molecular Mechanism of Thermal Noise in Rod Photoreceptors.*  
Gozem S., Schapiro I, Ferré N, Olivucci M  
**Midwest Theoretical Chemistry Conference (MWTCC)**, Urbana-Champaign, IL. **2013.**

## Posters

8. *Total and Differential Cross Sections of Open-Shell Species from Equation-of-Motion Coupled-Cluster Dyson Orbitals.*  
Gozem S., Krylov AI  
**ACS National Meeting**, Philadelphia, PA. **2016.**
7. *Photoelectron Wave Function in Photoionization: Plane Wave or Coulomb Wave?*  
Gozem S., Osborn DL, Stanton JF, Krylov AI  
**Pacific Conference on Spectroscopy and Dynamics**, Pacific Grove, CA. **2016.**
6. *Photoelectron Spectra and Photoelectron Angular Distributions From Equation-of-Motion Coupled-Cluster Dyson Orbitals.*  
Gozem S., Krylov AI  
**Photochemistry Gordon Research Conference**, Easton, MA. **2015.**
5. *Photoionization of Water in Gas Phase and in Bulk: Insight From Equation-of-Motion Coupled-Cluster Dyson Orbitals.*  
Gozem S., Krylov AI  
**ACS National Meeting**, Denver, CO. **2015.**
4. *Photodetachment and Photoionization Cross-Sections from Equation-of-Motion Coupled-Cluster Dyson Orbitals.*  
Gozem S., Gunina A, Krylov AI  
**2014 Conference on Excited State Processes**, Santa Fe, NM. **2014.**
3. *Effect of Dynamic Electron Correlation on a CASSCF Potential Energy Surface with Varying Covalent and Charge Transfer Electronic Characters.*  
Gozem S., Huntress M, Schapiro I, Lindh R, Granovsky AA, Angeli C, Olivucci M  
**ACS National Meeting**, Philadelphia, PA. **2012.**
2. *Molecular Mechanism of the Dark Noise in Rod Photoreceptors.*  
Gozem S., Schapiro I, Ferré N, Olivucci M  
**ACS National Meeting**, Denver, CO. **2011.**
1. *Retinal in Rhodopsin Can Thermally Isomerize via Two Competing Transition States.*  
Gozem S., Schapiro I, Ferré N, Olivucci M  
**ACS National Meeting**, Denver, CO. **2011.**

## Other Synergistic Activities

Reviewed manuscripts for the following journals:

- Chemical Reviews (ACS)
- Topics in Current Chemistry (Springer)
- Chemistry - A European Journal (Wiley)
- Chemistry - An Asian Journal (Wiley)
- Journal of Chemical Theory and Computation (ACS)
- Physical Chemistry Chemical Physics (RSC)
- ChemPhysChem (Wiley)
- Chemical Physics Letters (Elsevier)
- Molecular Physics (Taylor & Francis)
- Computational and Theoretical Chemistry (Elsevier)
- Heterocyclic Communications (De Gruyter)
- Computational Biology and Chemistry (Elsevier)