

SAMER GOZEM, PH.D
CURRICULUM VITAE

Department of Chemistry
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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.

Scholarship

Computational Support at National Supercomputing Facilities

2018-2019 NSF/XSEDE program CHE180027. *Insight into Structure-Function Relations in Light-Oxygen-Voltage (LOV) proteins.* Award size: 500,000 CPU hours (estimated value \$7,933.16)

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](#).

Mentoring

Postdoctoral Research Scholars

1. Yoelvis Orozco-Gonzalez (2017 – present)

Graduate Students

4. Nicole Ogbomoh (M.S., 2018 – present)
3. Md Mahbub (M.S., 2018 – present)
2. Rebecca Johnson (dual degree B.S./M.S., 2018 – present, LSAMP awardee)
1. Mohammad Pabel Kabir (Ph.D., 2017 – present)

Undergraduate and Post-Baccalaureate Students

4. Anah Wynn (2018 – present)
3. Andy Nguyen (2018)
2. Emrah Trumic (2018)
1. Atif Niaz (PostBacc, 2017-2018)

Teaching

Physical Chemistry I (CHEM 4110, CHEM 6110), **Physical Chemistry Problem I** (CHEM 4111).
Physical Chemistry II (CHEM 4120, CHEM 6120).
Biophysical Chemistry (Co-taught, Chem 8510).
Directed Research and Laboratory courses (CHEM 4160, CHEM 4170, CHEM 8910, CHEM 8999)

Conferences and Workshops

Invited Talks

3. *Shedding Light on Proteins with Computers*
Orozco-Gonzalez Y, Kabir MP, [Gozem S](#)
Scientific Computing Day, Georgia State University, Atlanta, GA. **2018**.
2. *Average electrostatic approach for multi-configurational QM/MM.*
Orozco-Gonzalez Y, Kabir MP, [Gozem S](#)
Atlanta Mini Symposium on Theoretical and Computational Chemistry, Emory University, Atlanta, GA. **2018**.
1. *Average electrostatic approach for multi-configurational QM/MM.*
Orozco-Gonzalez Y, Kabir MP, [Gozem S](#)
Developments in QM/MM and Embedding Models for Photochemical and Electron Transfer Processes, Telluride Science Research Center, Telluride, CO. **2018**.

Contributed Talks at National Conferences

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 Presented at National Conferences

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.**

Local Talks / Outreach

8. *Quantum and hybrid quantum/classical calculations on flavoproteins.*
Atlanta Flavin Meeting, GSU, Atlanta, GA. **Oct. 2018.**
7. *Shedding Light on Proteins with Computers.*
Middle Georgia State University Undergraduate Conference, Macon, GA. **Apr. 2018.**
6. *Starting a Career in Academia: Reflections and Impressions.*
Undergraduate STEM Research Society at GSU, Atlanta, GA. **Mar. 2018.**
5. *Starting a Career in Academia: Reflections and Impressions.*
Tri-Beta GSU, Atlanta, GA. **Feb. 2018.**
4. *What are orbitals and what can they tell us about biology?*
Chemistry Sophomore Research Seminar, GSU. Atlanta, GA. **Feb. 2018.**
3. *Are orbitals real? Two stories about seeing wave functions.*
ACS Middle Georgia Section Meeting, Macon, GA. **Jan. 2018.**
2. *Seeing Wave Functions: Modeling Photoelectron Spectra and Images in the Gas and Condensed Phase.*
Applied and Computational Math (ACM) Seminar at GSU, Atlanta, GA. **Nov. 2017.**
1. *Computational Photochemistry and Photobiology.*
Pizza Lunch with Chemistry Faculty, GSU, Atlanta, GA. **Sept. 2017.**

Synergistic Activities

Peer Review in Academic Journals

Reviewed a total of 28 articles in 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)