

SAMER GOZEM, PH.D
CURRICULUM VITAE

Department of Chemistry
P.O. Box 3965
Atlanta, GA 30302-3965

Phone: (404)413-5569
Email: sgozem@gsu.edu
Google Scholar profile: [Link](#)

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

2021 – present Associate Director of Graduate Studies.

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

2014 – 2017 Postdoctoral Research. University of Southern California.
Advisor: Prof. Anna I. Krylov

Awards

2021 Dean’s Early Career Award, GSU.

2021 National Science Foundation CAREER award.

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.

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

Scholarship

Research Funding

2021 – 2026 National Science Foundation (NSF) CAREER Grant CHE-2047667. *CAREER: Shedding light on the Photochemistry of the LOV Class of Flavin Photoreceptors*. Role: Principal Investigator. Total award: \$698,430 (\$419,058 obligated to date).

2020 – 2022 American Chemical Society Petroleum Research Fund (PRF) Doctoral New Investigator (DNI) Grant. *Calculation of Photoelectron Circular Dichroism of Small Chiral Organic Molecules*. Role: Principal Investigator. Total award: \$110,000.

2020 Georgia State University Molecular Basis of Disease SEED grant. *Protein Control of Flavin Redox Properties in Flavoproteins: A Combined Computational, Mutagenesis, and Spectroscopic Study*. Role: Co-PI with Drs. Gary Hastings and Giovanni Gadda. Total award: \$25,000.

2019 – 2020 Cleon C. Arrington Research Initiation Grant. *Insight into Structure-Function Relations in Light-Oxygen-Voltage (LOV) proteins*. Role: Principal Investigator. Total award: \$20,000.

Computational Support at National Supercomputing Facilities

2020 – 2021 NSF/XSEDE Educational allocation CHE180069. *Chem 4160 - Chemistry Laboratory (Computational)*. Award size: 24,000.0 CPU hours (estimated value \$396.40)

2020 – 2021 NSF/XSEDE program CHE180027. *Computational Modeling of Light-Induced Processes in Organic Molecules*. Award size: 300,000.0 CPU hours (estimated value \$4,682.00)

2019 – 2020 NSF/XSEDE program CHE180027. *Insight into Structure-Function Relations in Light-Oxygen-Voltage (LOV) proteins*. Award size: 227,851.0 CPU hours (estimated value \$3,690.77)

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)

Internal Computational Support

2021 – 2022 ARCTIC research allocation. *Electrostatic Tuning Maps and Average Electrostatic Configurations for Studying Flavoproteins*. Award: 700,000.0 CPU hours and 18,000 GPU hours.

Publications

Journal Articles

42. *Recipes for Simulating Photoelectron Circular Dichroism*
Gozem S, Garcia-Alvarez JC.
Submitted 2021.
41. *OS100: A Benchmark Set of 100 Digitized UV-Visible Spectra and Derived Experimental Oscillator Strengths*
Tarleton AS, Garcia-Alvarez JC, Wynn A, Awbrey CM, Roberts TP, Gozem S.
J. Phys. Chem. A. Article ASAP. 2022. [Link to Article](#).
40. *The Ionic Atmosphere Effect on the Absorption Spectrum of a Flavoprotein: A Reminder to Consider Solution Ions*
Dratch BD, Orozco-Gonzalez Y, Gadda G, Gozem S.
J. Phys. Chem. Lett. 12 (34), 8384–8396. **2021.** [Link to Article](#).
39. *Tuning Protein Dynamics to Sense Rapid Calcium Dynamics*
Deng X, Yao X, Berglund K, Dong B, Ouedraogo D, Ghane MA, Zhuo Y, McBean C, Wei ZZ, Gozem S, Yu SP, Wei L, Fang N, Mabb AM, Gadda G, Hamelberg D, Yang JJ.
Angew. Chem. Int. Ed. 60 (43), 23289–23298. **2021.** [Link to Article](#).

38. *Free Energy Computation for an Isomerizing Chromophore in a Cavity via the Average Solvent Electrostatic Configuration Model: Application to Rhodopsin and Rhodopsin-mimicking Systems*
Nikolaev D, Madushanka M, Orozco-Gonzalez Y, Shtyrov A, Guerrero-Martinez Y, [Gozem S](#), Ryazantsev M, Coutinho K, Canuto S, Olivucci M.
J. Chem. Theory Comput. 17(9), 5885–5895. 2021. [Link to Article](#).
37. *The effect of hydrogen-bonding interactions on the infrared vibrational spectrum of flavin*
Kabir MP, Orozco-Gonzalez Y, Hastings G, [Gozem S](#).
Spectrochim. Acta A. 911(1), 120110, 2021. [Link to Article](#).
36. *The ezSpectra Suite: An easy-to-use Toolkit for Spectroscopy Modeling*
[Gozem S](#), Krylov, AI.
WIREs Comput. Mol. Sci. e1546. 2021. [Link to Article](#).
35. *Cyclopropenone (c-C₃H₂O) as a Tracer of the Non-Equilibrium Chemistry Mediated by Galactic Cosmic Rays in Interstellar Ices*
Kleimeier NF, Abplanalp MJ, Johnson RN, [Gozem S](#), Wandishin J, Shingledecker CN, Kaiser RI.
Astrophys. J. 262(1), 24, 2021. [Link to Article](#).
34. *A Single Point Mutation in D-Arginine Dehydrogenase Unlocks a Transient Conformational State Resulting in Altered Cofactor Reactivity*
Iyer I, Reis RAG, Gannavaram S, Momin M, Spring-Connell AM, Orozco-Gonzalez Y, Agniswamy J, Hamelberg D, Weber IT, [Gozem S](#), Wang S, Germann MW, Gadda G.
Biochemistry 60(9), 711–724. 2021. [Link to Article](#).
33. *QM/MM Investigation of the Spectroscopic Properties of the Fluorophore of Bacterial Luciferase*
Giuliani G, Melaccio F, [Gozem S](#), Cappeli A, Olivucci M.
J. Chem. Theory Comput. 17(2) 605–613. 2021. [Link to Article](#).
32. *Probing the Electronic Structure of Bulk Water at the Molecular Length Scale with Angle-Resolved Photoelectron Spectroscopy*
[Gozem S](#), Seidel R, Hergenhan U, Lugovoy E, Abel B, Winter B, Krylov AI, Bradforth SE.
J. Phys. Chem. Lett. 11(13) 5162–5170. 2020. [Link to Article](#).
- Cover feature on J. Phys. Chem. Lett. [Link to Cover](#).
31. *Excited state vibronic dynamics of bacteriorhodopsin from 2D electronic photon echo spectroscopy and multi-configurational quantum chemistry*
[Gozem S](#), Johnson PJM, Halpin A, Luk HL, Morizumi T, Prokhrenko VI, Ernst OP, Olivucci M, Miller RJD.
J. Phys. Chem. Lett. 11(10) 3889–3896. 2020. [Link to Article](#).
30. *Electronic Spectra of Flavin in Different Redox and Protonation States: A Computational Perspective on the Effect of the Electrostatic Environment*
Kabir MP, Orozco-Gonzalez Y, [Gozem S](#).
Phys. Chem. Chem. Phys. 21, 16526–16537. 2019. [Link to Article](#).
29. *Electrostatic Spectral Tuning Maps for Biological Chromophores*
Orozco-Gonzalez Y, Kabir MP, [Gozem S](#).
J. Phys. Chem. B. 148, 4813–4824. 2019. [Link to Article](#).
- Featured as a front cover. [Link to Issue](#).

28. *Fluorescence Properties of Flavin Semiquinone Radicals in Nitronate Monooxygenase*
Su D, Kabir MP, Orozco-Gonzalez Y, [Gozem S](#), Gadda G.
ChemBioChem, 148, 1646–1652. 2019. [Link to Article](#).
- Cover feature on ChemBioChem. [Link to Cover](#).
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](#).

Book Chapter

Computational Photochemistry and Photobiology.

EI-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.; Third edition. CRC press: USA, 2012. [Link to Chapter](#).

Mentoring

Postdoctoral Research Scholars

2. Dr. Paulami Ghosh (2022 – present)
1. Dr. Yoelvis Orozco-Gonzalez (2017 – 2021)

Ph.D. Students

2. Jorge Garcia Alvarez (Ph.D., Molecular Basis of Disease Fellow, 2019 – present)
1. Mohammad Pabel Kabir (Ph.D., Molecular Basis of Disease Fellow, 2017 – present)

M.S. Students

7. Ngan Le (M.S., 2021 – present)
6. Astrid Tarleton (B.S/M.S., 2019 – 2021)
5. Mohammadnabi Ilanikashkouli (M.S., 2019 – 2021)
4. Nicole Ogbomoh (M.S., 2018 – 2021)
3. Nicolas Zemel (M.S., 2019 – 2020)
2. Md Mahbub (M.S., 2018 – 2020)
1. Rebecca Johnson (dual degree B.S./M.S., LSAMP awardee, 2018 – 2019)

List of student awards

12. Jorge C. Garcia-Alvarez (2021 – present): MBD PhD Fellowship.
11. Mohammad Pabel Kabir (2021): Harry P. Hopkins, Jr. Scholarship in Physical Chemistry
10. Astrid Tarleton (2021): Graduate Teaching Award
9. Mohammad Pabel Kabir (2021): MBD Outstanding Fellow Award
8. Md Mahbub (2020): Chemistry Master's Gold Award
7. Rebecca Johnson (2020): Graduate Teaching Award
6. Mohammad Pabel Kabir (2019 – present): MBD PhD Fellowship
5. Xuan Nguyen (2019): MBD Summer Undergraduate Fellowship
4. Rebecca Johnson (2019): Excellence in Undergraduate Work Award
3. Rebecca Johnson (2019): Excellence in Teaching Assistance Award
2. Rebecca Johnson (2018): LSAMP Fellowship
1. Atif Niaz (2018): Poster award at First Annual Greater Atlanta Chemical Biology Symposium.

Teaching

Thermodynamics and Chemical Kinetics (CHEM 4110, CHEM 6110, CHEM 4111).
Quantum and Statistical Mechanics (CHEM 4120, CHEM 6120).
Photophysics, Photochemistry, and Photobiology (CHEM 4470, CHEM 6470).
Seminar in Chemistry (CHEM 4940, CHEM 8800).
Biophysical Chemistry (Co-taught, Chem 8510).
Directed Research and Laboratory courses (CHEM 4160, CHEM 4170, CHEM 4950, CHEM 8910, CHEM 8999)

Conferences and Workshops

Invited Talks

10. *Ionic Atmosphere Effects: A Reminder to Consider Solution Ions in Computational Simulations*
Gozem S
2021 Southeastern Regional Meeting of the ACS (SERMACS), Birmingham, AL. 2021.
9. *Simulation of UV-visible spectra*
Gozem S
Department of Chemistry Seminar at College of Charleston, Charleston, SC. 2021.
8. *Electrostatic Tuning Maps and Average Protein Configurations: Strategies to Aid in Studying Flavoproteins*
Gozem S
The 20th International Symposium on Flavins and Flavoproteins, Graz, Austria. 2021.

7. *The ezSpectra Suite: An easy-to-use Toolkit for Spectroscopy Modeling*
Gozem S
Q-Chem Webinar, Online. 2021. [Link to Recording](#).
6. *Computational Photoelectron Spectroscopy: Theory and Applications to Bulk Water and Interstellar Organic Molecules*
Gozem S
Department of Physics and Astronomy Colloquium at GSU, Atlanta, GA. 2020.
5. *Spectral Tuning Maps and Average Protein Configurations: Strategies to Aid in Studying Flavoproteins*
 Orozco-Gonzalez Y, Kabir MP, Gozem S
2019 Southeastern Regional Meeting of the ACS (SERMACS), Savannah, GA. 2019.
4. *Spectral Tuning Maps and Average Protein Configurations: Strategies to Aid in Studying Flavoproteins*
 Orozco-Gonzalez Y, Kabir MP, Gozem S
2019 Southeast Theoretical Chemistry Association (SETCA), Knoxville, TN. 2019.
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

10. *The Average Protein Electrostatic Configuration Approach and its Application to Flavoproteins.*
 Yoelvis Orozco-Gonzalez, M. Pabel Kabir, Gozem S.
ACS National Meeting, Atlanta, GA. 2021 (virtual talk).
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.**

Synergistic Activities

Conferences and Workshops Organized

2. **2021 Atlanta Symposium on Computational and Theoretical Chemistry.**
 Georgia State University, Atlanta, GA. **Oct 2021.**
1. **Developments in QM/MM and Embedding Models for Photochemical and Electron Transfer Processes.**
Postponed to 2023 due to COVID-19. Was scheduled for July 2020 in Telluride, CO, but is postponed to 2023. Instead, I helped organize and host two online talks as part of the Telluride Science Summer Lecture Series.
 Telluride Science Research Center, Telluride, CO. **Oct 2020.**
 Co-organized with Profs. Lyudmila Slipchenko and Debashree Ghosh.

Peer Review in Academic Journals

Peer reviewed articles in the following journals:

- Nature Communications (Nature)
- Scientific Reports (Nature)
- Chemical Reviews (ACS)
- Journal of Chemical Theory and Computation (ACS)
- Journal of Physical Chemistry Letters (ACS)
- Journal of Physical Chemistry B (ACS)
- Journal of Physical Chemistry A (ACS)
- Journal of Chemical Information and Modeling (ACS)
- Topics in Current Chemistry (Springer)
- Challenges and Advances in Computational Chemistry and Physics (Springer)
- Physical Chemistry Chemical Physics (RSC)
- Journal of Chemical Physics (AIP)
- Chemistry - A European Journal (Wiley)
- Chemistry - An Asian Journal (Wiley)
- ChemPhysChem (Wiley)
- Molecular Physics (Taylor & Francis)
- Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy (Elsevier)
- Chemical Physics Letters (Elsevier)
- Computational and Theoretical Chemistry (Elsevier)
- Computational Biology and Chemistry (Elsevier)
- Heterocyclic Communications (De Gruyter)

- International Journal of Molecular Sciences (MDPI)
- Frontiers in Chemistry (Frontiers Media)
- Frontiers in Science, Technology, Engineering and Mathematics.

Grant Peer Reviews

Reviewed grants for following agencies:

- National Science Foundation (NSF), **ad hoc reviewer**.
- National Science Foundation (NSF), **panelist**.
- European Research Council (ERC), **external reviewer**.
- University Research Board (URB) of the American University of Beirut (AUB), **reviewer**.