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), Lebanon.

International Baccalaureate (IB) Diploma (2005), ICARDA International School of Aleppo, Syria.

Professional Experience

Director of Graduate Studies (**2025 – present**), Chemistry, Georgia State University.

Associate Professor of Chemistry (**2023 – present**). Georgia State University.

Associate Director of Graduate Studies (**2021 – 2024**), Chemistry, Georgia State University.

Assistant Professor of Chemistry (**2017 – 2023**). Georgia State University.

Postdoctoral Researcher (**2014 – 2017**). University of Southern California.
Advisor: Prof. Anna I. Krylov

Awards

2021 Dean's Early Career Award, GSU.
2021 National Science Foundation CAREER award.
2021 Awarded merit-based course release for Spring 2022 through PAWS Jr., GSU.
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 First Academic Award, Department of Chemistry, AUB

Scholarship

Research Funding

2023 – 2026 Department of Energy Basic Energy Science (BES) Energy Earthshot Research Center. DESC0024716. *Atomic Level Compositional Complexity for Electrocatalysis (Atomic-C2E).* Role: Co-PI with Gangli Wang et al. Total award: $2,550,000 (shared by all team members).

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.

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.

Current Computational Support at Supercomputing Facilities

2023 – 2025 NSF ACCESS program CHE180027. *Benchmarking Excited-State Quantum Chemical Methods Beyond the Vertical Excitation Energy*. 200,000 CPU hours (estimated value $465)

2023 – 2025 ARCTIC research allocation. *Ground and Excited-State Redox Potentials in Flavoproteins from Hybrid Quantum/Molecular Mechanical Models*. Award: 800,000.0 CPU hours and 25,000 GPU hours.

Previous Computational Support at Supercomputing Facilities

2018 – 2023 NSF/XSEDE program research allocation CHE180027. Renewed twice. Award (total over four years): 1,027,851 CPU hours (estimated value $16,305)

2021 – 2023 ARCTIC research allocation. *Electrostatic Tuning Maps and Average Electrostatic Configurations for Studying Flavoproteins*. Award: 700,000.0 CPU hours and 18,000 GPU hours.

2018 – 2021 NSF/XSEDE educational allocation CHE180069. Renewed twice. Award (total over three years): 79,000.0 CPU hours (estimated value $1,585)

Publications

Total citations: 2696. **Since 2019:** 1822. **H-index:** 28. **I10-index:** 41. **Date last updated:** 01/06/2025.
Source: Google Scholar profile page.

Corresponding or co-corresponding authorship** is indicated with ***.
Equal contribution first authorship** is indicated with **#.
***Authors from my lab** are underlined.*
Undergraduate students from my lab** are indicated with **†.
Dual degree BS/MS students** who started research in my lab as undergraduate students are indicated with **‡.
Articles below are listed from newest to oldest

Preprints

57. *The path to the triplet state in LOV domains.*
Ghosh P, Ajagbe SO, Gozem S*
ChemRxiv. This content is a preprint and has not been peer-reviewed yet. Link to Preprint.

Journal Articles

56. *Teaching Nonradiative Transitions with MATLAB and Python.*
Zheng X, Drummer MC, Russell TA, Gozem S, Glusac KD*
J. Chem. Ed. *101(11)*, 5097–5104, **2024**. Link to Article.

55. *Facile interconversion of mesitylcopper into a CuMes–Cu2bis(amidinate) triangle and a tetracuprous Möbius strip.*
Dowling K, Kruczyński T, Dutta S, Le DPN, Gozem S, McMillen CD, Bhuvanesh CD, Stollenz M*
Chem. Comm. *60(79)*, 11136–11139, **2024**. Link to Article.

54. *Absorption Intensities of Organic Molecules from Electronic Structure Calculations versus Experiments: the Effect of Solvation, Method, Basis Set, and Transition Moment Gauge.*
Garcia-Alvarez JC,* Gozem S*
J. Chem. Theory Comput. *20(16),* 7227–7243, **2024**. Link to Article.

53. *Electronic Structure Methods for Simulating Flavin's Spectroscopy and Photophysics: Comparison of Multi-reference, TD-DFT, and Single-Reference Wave Function Methods*
Kabir MP, Ghosh P, Gozem S*
J. Phys. Chem. B. *128(31)*, 7545–7557, **2024**. Link to Article.

52. *First and Second Reductions in an Aprotic Solvent: Comparing Computational and Experimental One-Electron Reduction Potentials for 345 Quinones*
Elhajj S, Gozem S*
J. Chem. Theory Comput. *20(14)*, 6227–6240, **2024**. Link to Article.

51. *Twisted and Disconnected Chains: Flexible Linear Tetracuprous Arrays and a Decanuclear Cu^{I} Cluster as Blue- and Green/Yellow-Light Emitters*
Arras J, Calderón-Díaz A, Lebedkin S, Gozem S, McMillen CD, Bhuvanesh N, Stollenz M*
Inorg. Chem. *63(28),* 12943–12957 **2024.** Link to Article.

50. *Solvent-Dependent Emissions Properties of a Model Aurone Enable Use in Biological Applications*
Anderson B, Bryant DL, Gozem S, Brambley C, Handy ST, Farone A, Miller JM*
J. Fluoresc. *In press.* **2024.** Link to Article.

49. How Aqueous Solvation Impacts the Frequencies and Intensities of Infrared Absorption Bands in Flavin: The Quest for a Suitable Solvent Model.
Le DPN, Hastings G, Gozem S*.
Molecules *29(2)*, 520. **2024.** Link to Article.

48. Solvatochromic and aggregation-induced emission active nitrophenyl-substituted pyrrolidinone fused-1,2-azaborine with a pre-twisted molecular geometry
*Campbell AD, Ellis K, Gordon LK, Riley JE, Le VV, Hollister KK, Ajagbe SO, Gozem S, Hughley RB, Boswell AM, Adjei-sah O, Baruah PD, Whitt LM, Gilliard RJ, Saint-Louis CJ**
J. Mater. Chem. C. *11(40)*, 13740–13751. **2023.** Link to Article.

47. Synthesis and Evaluation of Cereblon-Recruiting HaloPROTACs
Ody BK, Zhang J, Nelson SE, Xie Y, Liu R, Dodd CJ, Jacobs SE, Whitzel SL, Williams LA, Gozem S, Turlington M,* Yin J*
ChemBioChem. *24(21)*, e202300498. **2023.** Link to Article.

46. Photoelectron Spectroscopy of Oppositely Charged Molecular Switches in the Aqueous Phase: Theory and Experiment
Ikonnikov E, Paolino M, Garcia-Alvarez JC, Orozco-Gonzalez Y, Granados C, Röder A, Léonard J, Olivucci M, Haacke S, Kornilov O,* Gozem S.*
J. Phys. Chem. Lett. *14(26)*, 6061–6070. **2023.** Link to Article.

45. An Alternative Strategy for Spectral Tuning of Flavin-binding Fluorescent Proteins.
Kabir MP, Ouedraogo D, Orozco-Gonzalez Y,* Gadda G,* Gozem S.*
J. Phys. Chem. B. *127(6)*, 1301–1311. **2023.** Link to Article.

44. Dipole Effects in the Photoelectron Angular Distributions of the Sulfur Monoxide Anion.
Ru B, Hart CA, Mabbs R, Gozem S, Krylov AI, Sanov A.*
Phys. Chem. Chem. Phys. *24,* 23367–23381. **2022.** Link to Article.

43. Photochemically Triggered Cheletropic Formation of Cyclopropenone (c-C_3H_2O) from Carbon Monoxide and Electronically Excited Acetylene
Wang J, Kleimeier NF, Johnson RN,‡ Gozem S,* Abplanalp MJ,Turner AM, Marks JH, Kaiser RI.*
Phys. Chem. Chem. Phys. *24,* 17449–17461. **2022**. Link to Article.
- Featured as part of the themed collection “2022 PCCP HOT Articles”. Link to Collection.
- Featured as a front-page back cover in PCCP. Link to Cover.

42. Quantum–classical simulations of rhodopsin reveal excited-state-population splitting and its effects on quantum efficiency.
Yang X, Manathunga M, Gozem S, Léonard J, Andruniów T, Olivucci M.*
Nat. Chem. *14*, 441–449. **2022**. Link to Article.

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. *126 (3),* 435–443. **2022.** Link to Article.

40. The ezSpectra Suite: An easy-to-use Toolkit for Spectroscopy Modeling
Gozem S,* Krylov, AI.*
WIREs Comput. Mol. Sci. *e1546*. **2021**. Link to Article.
- Recognized as a top cited paper in WIREs Comput. Mol. Sci. for 2022-2023.

39. *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.

38. *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.

37. *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.

36. *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.

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,# Hergenhahn 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.
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.; Third edition. CRC press: USA, **2012**. Link to Chapter.

Software and Computational Workflows

5. *Average Protein Electrostatic Configuration for Flavoproteins (APEC-F) v. 2.0* **(2024)**
Elhajj S, Ajagbe S, Orozco-Gonzalez Y, Kabir MP, Gozem S.
Role: Contributor and project administrator.
Link to Open-Source Software.

4. *Automated protocol for computing redox potentials* **(2024)**
Elhajj S, Gozem S.
Role: Project administrator.
Link to Open-Source Software.

3. *Web Electrostatic Spectral Tuning Maps (WebESTM) v. 1.0* **(2022)**
Gay J, Childress C, Orozco-Gonzalez Y, Kabir MP, Edirisinghe N, Gozem S.
Role: Contributor and project administrator.

2. *ezFCF v. 1.2.* **(2022)**
Wojcik P, Gozem S, Mozhayskiy V, Krylov AI.
Role: Contributor.
Link to Open-Source Software.
Link to User's Manual.

1. *ezDyson v. 5.0* **(2021)**
Gozem S, Krylov AI.
Role: Lead developer.
Link to Open-Source Software.
Link to User's Manual.

Conferences and Workshops

Invited Talks at International, National, Regional Conferences

25. *Connecting theory and experiments: Electronic transition strengths, photoelectron spectra, and redox potentials.*
2024 Southeastern Regional Meeting of the ACS (SERMACS). Atlanta, GA. **Oct 2024**.

24. *Electronic structure methods for simulating flavin's spectroscopy and photophysics.*
2024 Southeastern Regional Meeting of the ACS (SERMACS). Atlanta, GA. **Oct 2024**.

23. *The average protein electrostatic configuration (APEC) hybrid quantum mechanical / molecular mechanical approach: Recent applications*
2024 Southeastern Regional Meeting of the ACS (SERMACS). Atlanta, GA. **Oct 2024**.

22. *Flavoprotein Photoreceptors Through the Quantum Mechanical Looking Glass*
American Society for Photobiology 2024 Biennial Meeting. Chicago, IL. **Jul 2024**.

21. *Spectroscopy of Organic and Biological Systems: Connecting Theory and Experiments*
1st International Symposium on the Role of Organic, Medicinal & Pharmaceutical Chemistry in Small Molecules Discovery for Biomedical Applications. Cairo, Egypt (virtual). **Jun 2024**.

20. *Flavoproteins Through the Quantum Mechanical Looking Glass.*
28th Enzyme Mechanisms Conference. Naples, FL. **Jan 2024**.

19. *Electrostatic Tuning Maps and Average Protein Configurations: Tools to Aid in Studying Flavoproteins*
Scientific Computing Day @GSU. Atlanta, GA. **Nov 2023**.

18. *Spectroscopy in the Condensed Phase: Connecting Theory and Experiments*
10th Annual North Carolina Photochemistry Symposium. Charlotte, NC. **Oct 2023**.

17. *Spectroscopy in the Condensed Phase: Connecting Theory and Experiments*
Ohio Photochemical Society Meeting (OoPS). Oregon, OH. **Jul 2023**.

16. *Electrostatic Tuning Maps and Average Protein Configurations: Tools to Aid in Studying Flavoproteins*
Principles of light-induced charge transfer for optogenetics. Modena, Italy. **Jul 2023**.

15. *Average solvent electrostatic configuration QM/MM approach: Recent applications*
ACS National Meeting. Indianapolis, IN. **Mar 2023**.

14. *Spectroscopy in the Condensed Phase: Connecting Theory and Experiments.*
30th Inter-American Photochemical Society Meeting. Miramar Beach, FL. **Jan 2023**.

13. *Benchmarking Excited-State Quantum Chemical Methods: Oscillator Strengths and Potential Energy Surfaces*
10th Molecular Quantum Mechanics Conference. Blacksburg, VA. **2022**.

12. *Spectroscopy in the Condensed Phase: Connecting Theory and Experiments.*
2022 Southeast Theoretical Chemistry Association (SETCA). Atlanta, GA. ***2022***.

11. *Benchmarking Excited-State Quantum Chemical Methods: Oscillator Strengths and Potential Energy Surfaces*
ACS National Meeting. San Diego, CA. **2022.**

10. *Ionic Atmosphere Effects: Including Solution Ions in QM/MM Simulations*
ACS National Meeting. San Diego, CA. **2022.**

9. *Spectroscopy in the Gas and Condensed Phase: Bridging Theory and Experiments*
***Virtual Winter School on Computational Chemistry*.** Online. **2022.**

8. *The Average Solvent Electrostatic Configuration QM/MM Approach for Flavoproteins*
Sanibel Symposium, St. Simons Island, GA. **2022.**

7. *What We've Learned from Quantum Mechanical and QM/MM Calculations about Condensed-Phase Molecular Spectroscopy.*
Theory and Simulation of Electronic and Optical Processes in Molecules and Materials Seminar Series. Online. **2022**.

6. *Ionic Atmosphere Effects: A Reminder to Consider Solution Ions in Computational Simulations.*
2021 Southeastern Regional Meeting of the ACS (SERMACS). Birmingham, AL. **2021**.

5. *Electrostatic Tuning Maps and Average Protein Configurations: Strategies to Aid in Studying Flavoproteins*
The 20th International Symposium on Flavins and Flavoproteins, Graz, Austria. **2021.**

4. *The ezSpectra Suite: An easy-to-use Toolkit for Spectroscopy Modeling*
Q-Chem Webinar, Online. **2021.** Link to Recording.

3. *Spectral Tuning Maps and Average Protein Configurations: Strategies to Aid in Studying Flavoproteins*
2019 Southeastern Regional Meeting of the ACS (SERMACS), Savannah, GA. **2019.**

2. *Spectral Tuning Maps and Average Protein Configurations: Strategies to Aid in Studying Flavoproteins*
2019 Southeast Theoretical Chemistry Association (SETCA), Knoxville, TN. **2019.**

1. *Average electrostatic approach for multi-configurational QM/MM.*
Developments in QM/MM and Embedding Models for Photochemical and Electron Transfer Processes, Telluride Science Research Center, Telluride, CO. **2018.**

Invited Seminar Talks

16. *Flavoproteins Through the Quantum Mechanical Looking Glass*
Seminar at The University of Memphis. Memphis, TN. **Nov 2024.**

15. *Flavoproteins Through the Quantum Mechanical Looking Glass*
Seminar at Loyola University. Chicago, IL. **Sept 2024.**

14. *Computational Chemistry*
SciSynth (ARCTIC summer camp). Atlanta, GGA. **Jun 2024.**

13. *Spectroscopy in the Condensed Phase: Connecting Theory and Experiments*
Seminar at The University of South Dakota. Vermillion, SD. **Oct 2023.**

12. *The Average Solvent Electrostatic Configuration QM/MM Approach: Recent Applications*
Seminar at Università degli Studi di Siena. Siena, Italy. **June 2023.**

11. *Spectroscopy in the Condensed Phase: Connecting Theory and Experiments*
Seminar at Syracuse University. Syracuse, NY. **Mar 2023.**

10. *What We've Learned from Quantum Mechanical and QM/MM Calculations about Condensed-Phase Molecular Spectroscopy*
Seminar at Auburn University. Online. **Feb 2022.**

9. *Comparing UV-visible spectra from computations and experiments.*
***Department of Physics and Chemistry Seminar,* Clayton State University.** Online. **Feb 2022.**

8. *Simulation of UV-visible spectra*
Department of Chemistry Seminar at College of Charleston. Charleston, SC. **Oct 2021.**

7. *Computational Photoelectron Spectroscopy: Theory and Applications to Bulk Water and Interstellar Organic Molecules*
***Department of Physics and Astronomy Colloquium,* GSU.** Atlanta, GA. **Dec 2020.**

6. *Quantum and hybrid quantum/classical calculations on flavoproteins.*
Atlanta Flavin Meeting. GSU, Atlanta, GA. **Nov 2018.**

5. *Shedding Light on Proteins with Computers*
Scientific Computing Day. GSU, Atlanta, GA. **Oct 2018.**

4. *Average electrostatic approach for multi-configurational QM/MM.*
Atlanta Mini Symposium on Theoretical and Computational Chemistry. Emory University, Atlanta, GA. **Sept 2018.**

3. *Shedding Light on Proteins with Computers.*
Middle Georgia State University Undergraduate Conference. Macon, GA. **Apr 2018.**

2. *Are orbitals real? Two stories about seeing wave functions.*
ACS Middle Georgia Section Meeting. Macon, GA. **Jan 2018.**

1. *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.**

Contributed Talks (since 2017 only)

2. *Benchmarking Excited-State Quantum Chemical Methods: Oscillator Strengths and Potential Energy Surfaces.*
ACS National Meeting. San Diego, CA. **2022.**

1. *The Average Protein Electrostatic Configuration Approach and its Application to Flavoproteins.*
ACS National Meeting, Atlanta, GA. **2021** (virtual talk).

Contributed Poster Presentations (since 2017 only)

3. *Flavins Through the Quantum Mechanical Looking Glass*
21st International Flavins and Flavoproteins Symposium
Atlanta, GA. **Jul 2024.**

2. *Electrostatic Tuning Maps and Average Protein Configurations: Strategies to Aid in Studying Flavoprotein Photoreceptors.*
Gordon Research Conference on Photosensory Receptors and Signal Transduction.
Ventura Beach, CA. **Mar 2022.**

1. *Electrostatic Tuning Maps and Average Protein Configurations: Strategies to Aid in Studying Flavoproteins.*
7th Annual OpenMolcas Developers' Workshop. Minneapolis, MN. **Jun 2019.**

Mentoring

Postdoctoral Research Scholars

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

Ph.D. Students

5. Sarah Elhajj (Ph.D., 2023 – present)
4. Stephen Ajagbe (Ph.D., 2023 – present)
3. Ngan Le (Ph.D., Molecular Basis of Disease Fellow, 2023 – present)
2. Jorge Garcia Alvarez (Ph.D., Molecular Basis of Disease Fellow, 2019 – present)
1. Mohammad Pabel Kabir (Ph.D., Molecular Basis of Disease and Provost Dissertation Fellow, 2017 – 2023)

M.S. Students

12. Vy Vu (Thesis M.S., 2023 – present)
11. Tien Thai (Non-thesis M.S., 2023)
10. Jordan Gaines (Non-thesis M.S., 2022)
9. Stephen Ajagbe (Thesis M.S., 2022 – 2024)
7. Ngan Le (Thesis dual degree B.S./M.S., 2021 – 2024)
8. Wilson Lewis (Non-thesis M.S., 2021 – 2022)
6. Astrid Tarleton (Thesis M.S., 2020 – 2021)

5. Mohammadnabi Ilanikashkouli (Thesis M.S., 2019 – 2021)
4. Nicole Ogbomoh (Non-thesis M.S., 2018 – 2021)
3. Nicolas Zemel (Non-thesis M.S., 2019 – 2020)
2. Md Mahbub (Thesis M.S., 2018 – 2020)
1. Rebecca Johnson (Thesis dual degree B.S./M.S., LSAMP awardee, 2018 – 2019)

Undergraduate, Post-Baccalaureate, and High School Students

Below is the complete list of undergraduate (58), post-Baccalaureate (1), and high school students (2) involved in research. We trained those students on running quantum chemical calculations in a Unix environment. During the first half of the semester, projects typically involved running ground and excited-state quantum chemical calculations for organic dyes on a high-performance computing cluster. After that, we asked the students to develop an independent project with help from graduate lab members and discuss their computational results in the context of experimental literature in an end-of-semester report.
***Students who are co-authors on published articles** are **in bold**.*
***Students who presented posters or talks** are indicated with ¶.*
***Dual degree BS/MS students** are indicated with ‡.*
***Students who received awards for their research work** are indicated with §*

62. Isaac Bare (Spring 2024-present)
61. Jade Kang (UAP scholar, Fall 2023)
60. Matan Chester (Fall 2023 - Spring 2024)
59. Arya Rao (Fall 2023)
58. Mairi Allen (Summer 2023)
57. Khoi Dang (Summer 2023)
56. Henry Lefkowitz (UAP scholar, Summer 2023 – Spring 2024) ¶
55. Cristian Auh (Fall 2022 – 2023)
54. Tien Thai (Fall 2022) ¶
53. Ky-Quan Nguyen (Fall 2022)
52. Erica Browne (Spring 2022 – 2023) ¶ §
51. John (Tommy) Tapp (NSF-REU, Summer 2022) ¶ §
50. Mohamad Many Alo (Summer 2022)
49. James Gay (Spring 2021 – Summer 2022) ¶ §
48. Ngan Le (Fall 2021 – present) ¶ ‡
47. Britton Lewis (Fall 2021– Spring 2022)
46. Jedidiahy Hailu (Fall 2021)
45. An Pham (Fall 2021)
44. Brennan Kellner (Fall 2021)
43. Omari Greene (Fall 2021)
42. Zahraa Fakhri (Fall 2021)
41. Golden Chen (Fall 2021)
40. Janyah Seymore (Summer 2021)
39. Jeanitha Wells (Summer 2021 – Fall 2021)
38. Devrin Turner (Summer 2021)
37. Adriana Sanchez (Summer 2021)
36. Sarah Alajwaa (Summer 2021)
35. Zachary Cable (Spring 2021)
34. Kelly Cao (Spring 2021)
33. Norma Vazquez (Spring 2021)
32. Manatsawani Mutasa (Spring 2021)
31. Nada Gebba (Spring 2021)
30. Inaara Khimani (Spring 2021)
29. Cameron Phelps (Spring 2021)
28. Daniel Garcia (Spring 2021)
27. Brittany Brown (Spring 2021)
26. Vijay Panthayi (Spring 2021)
25. Christensen Lucas (Spring 2021)
24. Kidus Chernet (Spring 2021)

23. Chaela Gray (Spring 2021)
22. Ashtyne Jones (Fall 2020)
21. Erin Nix (Fall 2020)
20. Tam-Huang Nguyen (Fall 2020)
19. Ky-Quan Nguyen (Fall 2020)
18. Thang Nguyen (Summer 2020)
17. Jasmine Hau (Summer 2020)
16. Jasmine Marie Davis (Summer 2020)
15. **Cade Awbrey** (Fall 2019 – Spring 2020)
14. **Astrid Tarleton** (Fall 2019) ¶ ‡ §
13. Vy Vu (Fall 2019)
12. Xuan Nguyen (MBD Summer Fellow, Summer 2019 – Fall 2019) ¶ §
11. **Tomas Roberts** (Spring 2019 – Fall 2019) ¶
10. Shelby Mendez (MBD "Catch Them Young" High School Student, Summer 2019) ¶
9. Christina Kiruba (MBD "Catch Them Young" High School Student, Summer 2019) ¶
8. Joshua Lee (Summer 2019)
7. Joanne Linares (Summer 2019)
6. **Anah Wynn** (Fall 2018 – Spring 2019) ¶
5. Audi Jeter (Spring 2019) ¶
4. Andy Nguyen (Fall 2018)
3. Emrah Trumic (Fall 2018)
2. **Rebecca Johnson** (Spring 2018 – Summer 2018) ¶ § ‡
1. Atif Niaz (Post-Baccalaureate, Fall 2017 – Summer 2018) ¶ §

List of student awards

24. Stephen Ajagbe (2024): Outstanding Talk award , CGSA symposium
23. Jorge C. Garcia-Alvarez (2024): Harry P. Hopkins, Jr. Scholarship in Physical Chemistry
22. Ngan Le (2023 – present): MBD PhD Fellowship
21. Erica Browne (2023): Al Baumstark Undergraduate Research Award
20. Erica Browne (2023): LSAMP best poster award.
19. Mohammad Pabel Kabir (2022): Provost's Dissertation Fellowship
18. Mohammad Pabel Kabir (2022): CGSA Spring Symposium Poster Award
17. James Gay (2022): ACS Award in Physical Chemistry
16. James Gay (2022): Al Baumstark Undergraduate Research Award
15. James Gay (2022): Robert H. Hankla Award
14. Erica Browns (2022): LSAMP Fellowship
13. Jorge C. Garcia-Alvarez (2021 – present): MBD PhD Fellowship
12. Mohammad Pabel Kabir (2021): Harry P. Hopkins, Jr. Scholarship in Physical Chemistry
11. Astrid Tarleton (2021): Graduate Teaching Award
10. Mohammad Pabel Kabir (2021): MBD Outstanding Fellow Award
9. James Gay (2021): LSAMP Fellowship
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

Courses Developed and Instructed at GSU

Photophysics, Photochemistry, and Photobiology (CHEM 4470, CHEM 6470). A 3-credit course that discusses events occurring in molecular systems following absorption of light. The course covers essential background concepts, how light absorption is accompanied by changes in molecular electronic and nuclear structure (photophysics), how such photophysical processes can lead to molecular transformations (photochemistry), and examples of photophysical and photochemical processes that occur in biological systems such as photoreceptor proteins and DNA (photobiology).

Courses Instructed at GSU

Thermodynamics and Chemical Kinetics (CHEM 4110, CHEM 6110)
Physical Chemistry Problem I (CHEM 4111).
Quantum and Statistical Mechanics (CHEM 4120, CHEM 6120).
Photophysics, Photochemistry, and Photobiology (CHEM 4470, CHEM 6470).
Responsible Conduct of Research (CHEM 6890).
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)

Educational Material and Labs Published Online

3. *MATLAB and Python scripts to teach nonradiative transitions* **(2024)**
   Developed by: Zheng X, Drummer MC, Russell TA, Gozem S, Glusac KD.
   Link to Scripts (see Supporting Information).

2. *Computing Franck-Condon Factors* **(2022)**
   Developed by: Garcia-Alvarez J and Gozem S. Edited by: Krylov AI.
   Link to Computational Lab.

1. *Molecular Orbitals of Diatomic Molecules in Their Lowest Singlet and Triplet States* **(2022)**
   Developed by: Tapp T, Gay Jr. JG, and Gozem S. Edited by: Krylov AI.
   Link to Computational Lab.

Service Activities

Conferences and Workshops Organizing Activities / Committees

4. ***75th Southeastern Regional Meeting of the American Chemical Society (SERMACS).***
   Oct 2024 in Atlanta, GA. **Oct 2024.**
   Member of organizing committee: Graduate fair chair and social media chair.
   Regional conference with attendance of over 2000 scientists and students.

3. ***21st International Flavins and Flavoproteins Symposium.***
   July 15-19, 2024, Georgia State University, Atlanta, GA. **July 2024**
   Co-chair of organizing committee with Giovanni Gadda.
   International conference with attendance of over 100 scientists and students.

2. ***2021 Atlanta Symposium on Computational and Theoretical Chemistry.***
   Organized at Georgia State University, Atlanta, GA. **Oct 2021.**

1. ***Developments in QM/MM and Embedding Models for Photochemical and Electron Transfer Processes.***
   Postponed to 2025 due to COVID-19. Was scheduled for July 2020 in Telluride, CO, but is postponed to 2024. 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:

- Angewandte Chemie International Edition (Wiley)
- Challenges and Advances in Computational Chemistry and Physics (Springer)
- Chemical Physics Letters (Elsevier)
- Chemical Reviews (ACS)
- Chemical Science (RSC)
- Chemistry - A European Journal (Wiley)
- Chemistry - An Asian Journal (Wiley)
- ChemPhysChem (Wiley)
- Computational and Theoretical Chemistry (Elsevier)
- Computational Biology and Chemistry (Elsevier)
- Frontiers in Chemistry (Frontiers Media)
- Frontiers in Science, Technology, Engineering and Mathematics.
- Heterocyclic Communications (De Gruyter)
- International Journal of Molecular Sciences (MDPI)
- Journal of the American Chemical Society (ACS)
- Journal of Chemical Information and Modeling (ACS)
- Journal of Chemical Physics (AIP)
- Journal of Chemical Theory and Computation (ACS)
- Journal of Enzyme Inhibition and Medicinal Chemistry (Taylor & Francis)
- Journal of Materials Chemistry C (RSC)
- Journal of Molecular Biology (Elsevier)
- Journal of Physical Chemistry A (ACS)
- Journal of Physical Chemistry B (ACS)
- Journal of Physical Chemistry Letters (ACS)
- Molecular Informatics (Wiley)
- Molecular Physics (Taylor & Francis)
- Molecules (MDPI)
- Nature Chemistry (Nature)
- Nature Communications (Nature)
- Physical Chemistry Chemical Physics (RSC)
- Proceedings of the National Academy of Sciences (National Academy of Sciences)
- Royal Society Open Science (RSC)
- Science Advances (AAAS)
- Scientific Reports (Nature)
- Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy (Elsevier)
- Topics in Current Chemistry (Springer)
- WIRES Computational Molecular Science (Wiley)

Grant Peer Reviews

Reviewed grants for following agencies:

- Department of Energy Office of Basic Sciences (DOE), **mail-in reviewer**.
- National Science Foundation (NSF), ***ad hoc* reviewer**.
- National Science Foundation (NSF), **panelist in two programs**.
- European Research Council (ERC), **external reviewer**.
- Petroleum Research Fund of the American Chemical Society (ACS), **reviewer**.
- University Research Board (URB) of the American University of Beirut (AUB), **reviewer**.

Duties as Associate Director of Graduate Studies in Chemistry (October 2021 – December 2024)

Oct 2021 – Dec 2024 Associate director of graduate studies in the Chemistry department. Activities:

- Formed a Committee with the goal to attract students to our graduate program and promote our department regionally and internationally.
- Chaired the Chemistry Graduate Admissions Committee.
- Faculty advisor to the Chemistry Graduate Student Association (CGSA).
- Organized orientations for incoming graduate students with the graduate director.
- Organized virtual open houses for prospective students.
- Other administrative duties.
  - I help maintain an accurate record of all our graduate students and their status.
  - I am the Chemistry department GPORT point of contact for graduate student hiring.

Committee and Panel Memberships in the Department of Chemistry, GSU

Nov 2024 – present Panel member for Department Specialist hire
Aug 2018 – Dec 2024 Chemistry Graduate Admissions Committee (Committee Chair as of Oct 2021).
Dec 2021 – Dec 2024 *Ad hoc* Department of Chemistry Branding Committee (Committee Chair).
Sept 2021 – Aug 2023 *Ad hoc* committee for developing a forensic chemistry concentration.
Aug 2021 – Feb 2022 Faculty Search Committee for two tenure-track assistant professor positions.
Aug 2018 – Apr 2022 Chemistry Curriculum Committee.

Committee Memberships outside of the Department of Chemistry, GSU

Aug 2023 – present Member of the Molecular Basis of Disease (MBD) Working Committee
Aug 2022 – present Associate coordinator, GA-AL Louis Stokes Alliance for Minority Participation (LSAMP) program at GSU.
Oct 2021 – present Member of the graduate council.
Mar 2021 – present Advanced Research Computing Technology and Innovation Core (ARCTIC) Governance Committee at GSU.
Aug 2023 – Oct 2023 Member of the Graduate Portal (GPORT) Enhancement Committee