# Gaurav Harsha

*Research Area Specialist Sr*

*Department of Chemistry*
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## Education

2016-2021 **Doctor of Philosophy**, *Physics and Astronomy*, Rice University, Houston, TX
Dissertation: Wave Function Theories For Finite-Temperature Electronic Structure

2016-2021 **Master of Science**, *Physics and Astronomy*, Rice University, Houston, TX

2011-2015 **Bachelor of Technology**, *Physical Science*, Gold medalist, Indian Institute of Space Science and Technology, Trivandrum, India

## Job and Research Experience

2025-present **Research Area Specialist Sr**, *Department of Chemistry*, University of Michigan, Ann Arbor, Core developer for the Green-Phys software package, leading implementations of new Green's function methods, training new users, and optimizing performance for modern HPC architectures.

2022-2025 **Postdoctoral Research Fellow**, *Department of Chemistry*, University of Michigan, Ann Arbor, Developed first-principles Green's function approaches for electronic structure of solid-state systems, with emphasis on relativistic effects, disorder, and topological phases.

2015-2016 **Scientist/Engineer**, *Space Applications Centre*, ISRO, Ahmedabad, Gujarat (India), Managed 24/7 thermal-vacuum lab operations, supervised staff, maintained equipment and budgets, and contributed to the design of a large-scale vacuum chamber

## Achievements

2025 **Best Poster Award**, "Describing Disorder and Correlation – Coherent Potential Approximation with Bloch Gaussians", at New Challenges for Ab-initio Theory in Molecular Sciences
Warsaw, Poland (July 1-5, 2025)

2019 **Journal of Chemical Physics Editor's Choice Paper**, "Thermofield Theory for finite-temperature quantum chemistry", J. Chem. Phys. 150, 154109 (2019)

2016 **Institute Gold Medal**, for outstanding academic performance, Indian Institute of Space Science and Technology, Trivandrum, Kerala (India)

2016 **Director's Gold Medal**, for best all-round performance, Indian Institute of Space Science and Technology, Trivandrum, Kerala (India)

## Professional Experience

Peer review American Physical Society: Phys. Rev. Lett., Phys. Rev. A & Phys. Rev. B

American Chemical Society: Journal of Chemical Theory and Computation

Royal Society of Chemistry: Physical Chemistry Chemical Physics

American Institute of Physics: APL Computational Physics

Mentor Undergraduate intern: Yi Xu (Zhejiang University, China); Project: *Finite-temperature Coupled Cluster for Spin Systems and Magnetic Properties*

Masters Intern: Selina Dirnbök (Vienna University of Technology); Project: *Band-structure investigation of topological $\alpha$-Sn and perovskite $BiVO_3$ using self-consistent GW*

Teaching Assistant — Fall 2018, 2019 & 2020; *Introduction to Quantum Chemistry* at Rice University; helped with designing and grading homework and exams; delivered selected lectures

## Selected Talks

July, 2025 **Frontiers in wave function and Green's function methods**, *Invited Seminar*, Department of Chemistry, University of Strasbourg, France

June, 2025 **Coherent potential approximation with Bloch Gaussian orbitals**, *Contributed Talk*, Numerical Methods in Quantum Chemistry, Berlin, Germany

May, 2025 **Finite-temperature coupled cluster theory**, *Invited Talk*, Flagship Workshop on Accurate methods for thermal and excited electrons, EPFL CECAM, Lausanne, Switzerland

May, 2025 **Exploring the phase diagram of $\alpha$-Sn using self-consistent GW**, *Contributed Talk*, 55th Midwest Theoretical Chemistry Conference, Wayne State University, Detroit, MI

July, 2024 **Challenges with relativistic GW calculations in solids and molecules**, *Contributed Talk*, Correlated electronic structure Faraday Discussion, Royal Society of Chemistry, London UK

March, 2023 **Effect of quasiparticle self-consistent schemes on the GW method**, *Contributed Talk*, APS March Meeting 2023, Las Vegas NV, USA

June, 2022 **Finite-temperature coupled cluster theory**, *Contributed Talk*, Midwest Theoretical Chemistry Conference, Ohio State University, Columbus, Ohio

## Publications

- **Harsha, G.**, Dirnbök, S., Vlček, V., Gull, E., & Zgid, D. Discovering topological phases in gray-Tin. *arXiv* 2511.22740 (2025)
- Reeves, C. C., **Harsha, G.** et al., Performance of wave function and Green's function based methods for non equilibrium many-body dynamics. Phys. Rev. Research 7, 023002 (2025)
- Iskakov, S., Yeh, C.-N., Pokhilko, P., **Harsha, G.** et al. `Green/WeakCoupling`: Implementation of fully self-consistent finite-temperature many-body perturbation theory for molecules and solids, *Comput. Phys. Commun.* 306 (2025) 109380
- **Harsha, G.**, Abraham, V. & Zgid, D. Quasiparticle and fully self-consistent $GW$ methods: an unbiased analysis using Gaussian orbitals. *Phys. Rev. B* 110, 235146 (2024)
- **Harsha, G.**, Abraham, V. & Zgid, D. Challenges with relativistic $GW$ calculations in solids and molecules. *Faraday Discuss.*, 2024, Advance Article (DOI: 10.1039/d4fd00043a)
- Abraham, V., **Harsha, G.** & Zgid, D. Relativistic fully self-consistent $GW$ for molecules: Total energies and ionization potentials. *J. Chem. Theory Comput.* 2024, 20, 11, 4579–4590
- Wen, M., Abraham, V., **Harsha, G.** et al., Comparing self-consistent $GW$ and vertex corrected $G_0W_0$ ($G_0W_0\Gamma$) accuracy for molecular ionization potentials. *J. Chem. Theory Comput.* 20, 3109 (2024)
- **Harsha, G.**, Henderson, T. M. & Scuseria, G. E. Thermofield theory for finite-temperature electronic structure. *J. Phys. Chem. A* 127 (14), 3063-3071 (2023)
- **Harsha, G.**, Xu, Y., Henderson, T. M. & Scuseria, G. E. Thermal coupled cluster theory for SU(2) systems. *Phys. Rev. B* 105, 045125 (2022)

- **Harsha, G.**, Henderson, T. M. & Scuseria, G. E. Wave function methods for canonical ensemble thermal averages in correlated many-fermion systems. *J. Chem. Phys.* 153, 124115 (2020)
- **Harsha, G.**, Henderson, T. M. & Scuseria, G. E. Thermofield theory for finite-temperature coupled cluster. *J. Chem. Theory Comput.* 15, 6127-6136 (2019)
- **Harsha, G.**, Henderson, T. M. & Scuseria, G. E. Thermofield theory for finite-temperature quantum chemistry. *J. Chem. Phys.* 150, 154109 (2019)
- **Harsha, G.**, Shiozaki, T. & Scuseria, G. E. On the difference between variational and unitary coupled cluster theories. *J. Chem. Phys.* 148, 044107 (2018)

## Programming Skills

Languages: Python, C++, Fortran, CUDA; Extensive experience with PySCF

Developer: https://green-phys.org: C++/Python packages for *ab initio* Green's function simulations; tfd-ccsd and canon-tfd: finite-temperature coupled cluster and perturbation theory packages; drudge: A symbolic algebra system for tensorial and noncommutative algebras

## Poster Presentations

July, 2025 **Coherent Potential Approximation with Bloch Gaussian Orbitals**, New Challenges for Ab-initio Theory in Molecular Science, Warsaw, Poland

June, 2025 **Coherent Potential Approximation with Bloch Gaussian Orbitals**, Congress of World Association of Theoretical and Computational Chemistry, Oslo, Norway

May, 2024 **Effect of self-consistency on the GW method**, Midwest Theoretical Chemistry Conference, University of Wisconsin, Madison

July, 2023 **Effect of self-consistency on the GW method**, International Congress of Quantum Chemistry, Bratislava, Slovakia

## Extra-curricular Activities

2018–2020 **President**, *Graduate Student Association Soccer Club*
Rice University, Houston, TX

2022–present **Member**, *Table Tennis Club*
University of Michigan, Ann Arbor, MI

2022–present **Member**, *Postdoctoral Association Soccer Club*
University of Michigan, Ann Arbor, MI

## References


- Prof. Dominika Zgid, University of Michigan, Ann Arbor, MI ✉ zgid@umich.edu
- Prof. Gustavo E. Scuseria, Rice University, Houston, TX ✉ guscus@rice.edu
- Prof. Vojtěch Vlček, University of California, Santa Barbara, CA ✉ vlcek@ucsb.edu
- Prof. Emanuel Gull, University of Michigan, Ann Arbor, MI ✉ egull@umich.edu