

# Gaurav Harsha

Research Area Specialist Senior

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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
- 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  $\text{BiVO}_3$  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

- June, 2026 **Exploring correlated topological materials using ab initio self-consistent GW**, *Contributed Talk*, International Congress on Quantum Chemistry, Berkeley (CA), USA
- 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

- Wen, M., **Harsha, G.** and Zgid, D., Dynamically Corrected Bethe-Salpeter Equation Solver for Self-consistent Reference on the Matsubara Frequency Axis. *arXiv* 2604.22187 (2026)
- **Harsha, G.**, Dirnbök, S., Vlcěk, 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  $G_0W_0$  ( $G_0W_0I$ ) 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)

## 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

## Programming Skills

- Languages Python, C++, Fortran, CUDA; Extensive experience with PySCF
- Products **GREEN-MBPT**: C++/Python packages for *ab initio* Green's function simulations;  
**GREEN-GPU**: CUDA accelerator for many-body methods used in GREEN-MBPT  
**TFD-CCSD** and **CANON-TFD**: finite-temperature coupled cluster and perturbation theory packages implemented using hybrid Python-Fortran framework;

## 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