

Gaurav Harsha

Computational & Theoretical Physicist

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Research Vision

I develop predictive, systematically improvable many-body methods that reach beyond the ground state to capture how electron correlation and its environment — finite temperature, disorder, and dissipation — shape correlated, topological, and open quantum systems, from molecules to materials. My interests span wavefunction and Green’s-function theories and their application across chemistry and condensed-matter physics.

Education

Ph.D., Physics & Astronomy **2016–2021**
Rice University, Houston, TX
Dissertation: *Wave Function Theories for Finite-Temperature Electronic Structure.*

M.S., Physics & Astronomy **2016–2021**
Rice University, Houston, TX (integrated with Ph.D.)

B.Tech., Physical Science (Gold Medalist) **2011–2015**
Indian Institute of Space Science & Technology, Trivandrum, India

Appointments

Research Area Specialist Senior **2025–present**
Department of Chemistry, University of Michigan, Ann Arbor
Lead development of the Green-Phys software package: implement new Green’s-function methods, onboard new users, and optimize performance for modern HPC architectures.

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

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

Honors & Awards

Best Poster Award **2025**
“Describing Disorder and Correlation: Coherent Potential Approximation with Bloch Gaussians”, New Challenges for Ab-initio Theory in Molecular Sciences, Warsaw

Editor’s Choice, J. Chem. Phys. **2019**
“Thermofield theory for finite-temperature quantum chemistry”, J. Chem. Phys. 150, 154109

Institute Gold Medal **2016**
Outstanding academic performance, Indian Institute of Space Science & Technology

Director’s Gold Medal **2016**
Best all-round performance, Indian Institute of Space Science & Technology

Teaching & Mentoring

- Mentoring** Co-supervised undergraduate intern Yi Xu (Zhejiang University): finite-temperature coupled cluster for spin systems; co-author, *Phys. Rev. B* **105**, 045125 (2022). Co-supervised Masters intern Selina Dirnböck (TU Wien): topological α -Sn via self-consistent GW; co-author, *arXiv:2511.22740* (2025). Both mentees have gone on to doctoral study.
- Teaching** Teaching Assistant, *Introduction to Quantum Chemistry*, Rice University (Fall 2018, 2019 & 2020): designed and graded homework and exams; delivered selected lectures
Laboratory Instructor (TA), introductory physics laboratory (engineering & pre-med), Rice University (4 semesters): ran lab sections, instructed students, and graded reports

Professional Service

- Peer review** American Physical Society (Phys. Rev. Lett., Phys. Rev. A & B); American Chemical Society (J. Chem. Theory Comput.); Royal Society of Chemistry (Phys. Chem. Chem. Phys.); American Institute of Physics (APL Computational Physics)

Invited Talks

- Frontiers in wave function and Green’s function methods** **Jul 2025**
Invited Seminar, Department of Chemistry, University of Strasbourg, France
- Finite-temperature coupled cluster theory** **May 2025**
Invited Talk, Flagship Workshop on Accurate Methods for Thermal and Excited Electrons, CECAM, EPFL, Lausanne, Switzerland

Contributed Talks

- Exploring correlated topological materials using ab initio self-consistent GW** **Jun 2026**
International Congress on Quantum Chemistry, Berkeley, CA, USA
- Coherent potential approximation with Bloch Gaussian orbitals** **Jun 2025**
Numerical Methods in Quantum Chemistry, Berlin, Germany
- Exploring the phase diagram of α -Sn using self-consistent GW** **May 2025**
55th Midwest Theoretical Chemistry Conference, Wayne State University, Detroit, MI
- Challenges with relativistic GW calculations in solids and molecules** **Jul 2024**
Correlated Electronic Structure Faraday Discussion, Royal Society of Chemistry, London, UK
- Effect of quasiparticle self-consistent schemes on the GW method** **Mar 2023**
APS March Meeting 2023, Las Vegas, NV, USA
- Finite-temperature coupled cluster theory** **Jun 2022**
Midwest Theoretical Chemistry Conference, Ohio State University, Columbus, OH

Publications

13 published articles and 2 preprints (9 first-author); *h*-index 11, 416 citations (Google Scholar, 2026). Author name in **bold**.

- **Harsha, G.**, Dirnböck, S., Gull, E., Vlcek, V. & Zgid, D. Symmetry-resolved topology from interacting Green’s functions. *arXiv:2511.22740* (2026).
- Yu, Y., **Harsha, G.** *et al.* Hybrid Hamiltonian-diagrammatic quantum impurity solver. *arXiv:2606.11095* (2026).
- Wen, M., **Harsha, G.** & Zgid, D. Dynamically corrected Bethe–Salpeter equation solver for a self-consistent reference on the Matsubara frequency axis. *J. Chem. Theory Comput.* **22**, 8257–8273 (2026).
- Reeves, C. C., **Harsha, G.** *et al.* Performance of wave function and Green’s function based methods for nonequilibrium 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**, 109380 (2025).
- **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), 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.* **20**, 4579–4590 (2024).
- 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**, 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). (*Editor’s Choice.*)
- **Harsha, G.**, Shiozaki, T. & Scuseria, G. E. On the difference between variational and unitary coupled cluster theories. *J. Chem. Phys.* **148**, 044107 (2018).

Selected Posters

Coherent Potential Approximation with Bloch Gaussian Orbitals	Jul 2025
<i>New Challenges for Ab-initio Theory in Molecular Science, Warsaw, Poland</i>	
Coherent Potential Approximation with Bloch Gaussian Orbitals	Jun 2025
<i>Congress of the World Association of Theoretical and Computational Chemistry, Oslo, Norway</i>	
Effect of self-consistency on the GW method	Jul 2023
<i>International Congress of Quantum Chemistry, Bratislava, Slovakia</i>	

Programming & Software

Languages	Python, C++, Fortran, CUDA; extensive experience with PySCF
Software	Green-Phys suite (green-phys.org): core developer of GREEN-MBPT/Green-WeakCoupling (C++/Python, <i>ab initio</i> Green’s-function simulations) and GREEN-GPU (CUDA accelerator for many-body methods). TFD-CCSD & CANON-TFD (thermal coupled cluster & perturbation theory, Python/Fortran, sole author)
Training	Onboarded 10–20 users of the Green-Phys suite across the group and collaborating institutions