# VIBIN ABRAHAM

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## PROFESSIONAL EXPERIENCE

**Postdoctoral Research Associate** *January 2022 - December 2024*
University of Michigan, Ann Arbor
Advisor: Prof. Dominika K. Zgid

- Application of self-consistent Green's function method for heavy element molecules and solids.

**Undergraduate Summer Researcher** *May 2014 - July 2014*
Virginia Tech, Blacksburg
Advisor: Prof. T. Daniel Crawford

- Investigated chiral imprint of an achiral solvent left by a chiral molecule in solution

## EDUCATION

**Ph.D in Chemistry** *August 2016 - December 2021*
Virginia Tech, Blacksburg
Advisor: Prof. Nicholas J. Mayhall
Dissertation: Modern Electronic Structure Theory using Tensor Product States

**Integrated Master's in Chemistry** *July 2011 - June 2016*
Indian Institute of Technology Bombay, Mumbai
Advisor: Prof. Raghavan B. Sunoj
Dissertation: Design of Asymmetric Catalysts using Multivariate Linear Regression

## PUBLICATIONS

**In Print**

1. **V. Abraham**, G. Harsha, and D. Zgid, Relativistic fully self-consistent *GW* for molecules: Total energies and ionization potentials, J. Chem. Theory Comput. **20**, 4579 (2024)
2. G. Harsha, **V. Abraham**, and D. Zgid, Challenges with relativistic *GW* calculations in solids and molecules, Faraday Discuss. (2024)
3. M. Wen, **V. Abraham**, G. Harsha, A. Shee, K. B. Whaley, and D. Zgid, 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)
4. A. Kumar, A. Asthana, **V. Abraham**, T. D. Crawford, N. J. Mayhall, Y. Zhang, L. Cincio, S. Tretiak, and P. A. Dub, Quantum simulation of molecular response properties in the NISQ era, J. Chem. Theory Comput. **19**, 9136 (2023)
5. N. M. Braunscheidel*, **V. Abraham***, and N. J. Mayhall, Generalization of the tensor product selected ci method for molecular excited states, J. Phys. Chem. A **127**, 8179 ( 2023)
6. A. Asthana, A. Kumar, **V. Abraham**, H. Grimsley, Y. Zhang, L. Cincio, S. Tretiak, P. A. Dub, S. E. Economou, E. Barnes, *et al.*, Quantum self-consistent equation-of-motion method for computing molecular excitation energies, ionization potentials, and electron affinities on a quantum computer, Chem. Sci. **14**, 2405 (2023)
7. **V. Abraham** and N. J. Mayhall, "Coupled electron pair-type approximations for tensor product state wave functions", J. Chem. Theory Comput. **18**, 4856 (2022)
8. **V. Abraham** and N. J. Mayhall, "Revealing the contest between triplet–triplet exchange and triplet–triplet energy transfer coupling in correlated triplet pair states in singlet fission", J. Phys. Chem. Lett. **12**, 10505 (2021)
9. **V. Abraham** and N. J. Mayhall, "Cluster many-body expansion: A many-body expansion of the electron correlation energy about a cluster mean field reference", J. Chem. Phys. **155** (2021)

10. **V. Abraham** and N. J. Mayhall, "Selected configuration interaction in a basis of cluster state tensor products", J. Chem. Theory Comput. **16**, 6098 (2020)
11. **V. Abraham** and N. J. Mayhall, "Simple rule to predict boundedness of multiexciton states in covalently linked singlet-fission dimers", J. Phys. Chem. Lett. **8**, 5472 (2017)
12. C. Patel,**V. Abraham**, and R. B. Sunoj, "Mechanistic insights and the origin of regioselective borylation in an Iridium-catalyzed alkyl C (sp3)–H bond functionalization", Organometallics **36**, 151 (2017)

**Preprint**

1. G. Harsha, **V. Abraham**, M. Wen, and D. Zgid, Quasiparticle and fully self-consistent *GW* methods: an unbiased analysis using gaussian orbitals, arXiv:2406.18077 (2024)
2. S. Iskakov, C.-N. Yeh, P. Pokhilko, Y. Yu, L. Zhang, G. Harsha, **V. Abraham**, M. Wen, M. Wang, J. Adamski, *et al.*, Green/weakcoupling: Implementation of fully self-consistent finite-temperature many-body perturbation theory for molecules and solids, arXiv:2406.18479 (2024)

* indicates equally contributing authors.

## TEACHING AND SERVICES

**General Chemistry** *Fall 2016, Spring 2017*
Graduate student instructor for undergraduate chemistry lab at Virginia Tech

**CH 105 (Introductory Organic Chemistry)** *Summer 2015*
Taught a batch of 100 students with a team of four Teaching Assistants during the summer term in IIT Bombay.

**Volunteer, Abhyasika** *August 2012 - August 2016*
Taught Maths and English grammar to underprivileged students from the informal settlement in Phoolenagar, Mumbai.

**Volunteer, LCWAA** *August 2020 - December 2020*
Taught chemistry to underprevileged high school students as part of LCCWA (Logic Centre and Community Welfare Association, Mumbai) during the COVID-19 lockdown.

**Reviewer** *July 2021 - Present*
Reviewer in Physical Review B (APS), Journal of Chemical Theory and Computation (ACS), Journal of Chemical Physics (AIP), Physical Chemistry Chemical Physics (RSC)

## AWARDS AND ACHIEVEMENTS

- **Best Postdoc Poster Award** *June 2022*
  52nd Midwest Theoretical Chemistry Conference (MWTCC)
- **Graduate Research Award** *2021*
  Department of Chemistry, Virginia Tech
- **IBM Zerner Graduate Student Award** *February 2020*
  60th Sanibel Conference
- **JCP Poster Award** *June 2018*
  16th International Congress of Quantum Chemistry (ICQC)
- **INSPIRE Scholarship** *July 2011- June 2016*
  Department of Science and Technology, Government of India
- Top 1 % in All India Rank in IIT-JEE 2011 competitive exam with more than 500,000 participants.

## PRESENTATION

1. Estimating the accuracy of pseudopotential based GW method at different levels of self consistency using Gaussian orbitals
   **V. Abraham**, M. Wen, G. Harsha and D. Zgid
   American Physical Society March Meeting, Las Vegas, Nevada, 2023

2. Modern electronic structure theory using tensor product states
   **V. Abraham** and N. J. Mayhall
   American Chemical Society National Meeting, Atlanta, Georgia, Spring 2021
3. Tensor Product Selected CI:Compact wave function for strongly correlated cluster-able systems
   **V. Abraham** and N. J. Mayhall
   Virtual Conference of Theoretical Chemistry, June 2020 [Graduate student Hon' Mention]

## SOFTWARE

- Green/weakcoupling package: Contributed to software framework for the simulation of realistic materials with Green's function methods.
- FermiCG: Contributed to development of the Julia package for fermionic many body problem by coarse-grained approaches.
- Adapt-VQE: Contributed to the simulation code of adapt-VQE and q-sc-EOM algorithms.

## REFERENCES

- **Professor Dominika K. Zgid**
  *zgid@umich.edu*
- **Professor Nicholas J. Mayhall**
  *nmayhall@vt.edu*
- **Professor T. Daniel Crawford**
  *crawdad@vt.edu*