Varun Rishi

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Education

- **University of Florida** — Gainesville, USA
  PhD, Prof. Rodney Bartlett, Chemistry, Quantum Theory Project — *2011 - 2017*

  Thesis: *In weak and in strong correlation: the search for a coupled cluster method that works in all scenarios*

- **Indian Institute of Science Education and Research** — Pune, India
  BS-MS — *2006 - 2011*

Work Experience

- **Sandia National Labs** — Livermore, USA
  Postdoctoral Researcher, Dr. Laura McCaslin, Combustion Research Facility — *2022 -*
- **California Institute of Technology** — Pasadena, USA
  Postdoctoral Researcher, Prof. Thomas Miller, Chemistry & Chemical Engineering — *2019 - 2020*
- **Virginia Tech** — Blacksburg, USA
  Postdoctoral Researcher, Prof. Edward Valeev, Chemistry — *2017 - 2019*

Research Grants

- **Principal Investigator, Laboratory Directed Research & Development Grant** — 2023
  DOE-Sandia National Lab Grant
  - *Towards efficient light emitters via computational design of molecules with inverted singlet-triplet gaps*

Publications

13. **Quantifying Design Principles for Light-Emitting Materials with Inverted Singlet–Triplet Energy Gaps**. Varun Rishi, Ali Abou Taka, Hrant Hratchian and Laura M. McCaslin. J. Phys. Chem. Lett. 16, 5213 (2025)
    doi:https://doi.org/10.1021/acs.jpclett.5c00827

12. **Excited State Electronic Structure of Dimethyl Disulfide Involved in Photodissociation at 200 nm**. Varun Rishi, Neil Cole-Filipiak, Krupa Ramasesha and Laura M. McCaslin. Phys. Chem. Chem. Phys. 6, 23986 (2024)

11. **Dark Doubly Excited States with Modified Coupled Cluster Models: A Reliable Compromise between Cost and Accuracy?**. Varun Rishi, Moneesha Ravi, Ajith Perera and Rodney J. Bartlett. J. Phys. Chem. A, 127, 828 (2023)

10. **Robust approximation of tensor networks: application to grid-free tensor factorization of the Coulomb interaction**. Karl Pierce, Varun Rishi and Edward F.Valeev. J. Chem. Theory Comput. 17, 4, 2217 (2021)

9. **Many-body quantum chemistry on massively parallel computers**. Justus Calvin, Chong Peng, Varun Rishi, Ashutosh Kumar and Edward F. Valeev . Chem. Rev. 121, 3, 1203 (2021)

8. **A route to improving RPA excitation energies through its connection to equation-of-motion coupled cluster theory**. Varun Rishi, Ajith Perera and Rodney J. Bartlett. J. Chem. Phys. 153, 234101 (2020)

7. **Massively Parallel Quantum Chemistry : A High-Performance Research Platform for Electronic Structure"**. Varun Rishi et al. J. Chem. Phys. 153, 044120 (2020)

6. **Can the distinguishable cluster approximation be improved systematically by including connected triples?**. Varun Rishi and Edward F. Valeev. J. Chem. Phys. 151, 064102 (2019)

5. **Behind the success of modified coupled-cluster methods: Addition by Subtraction**. Varun Rishi, Ajith Perera and Rodney J. Bartlett. Mol. Phys. 117:17, 2201 (2019)

4. **Excited states from modified coupled cluster methods: Are they any better than EOM CCSD?**. Varun Rishi, Ajith Perera, Marcel Nooijen and Rodney J. Bartlett. J. Chem. Phys. 143, 164103 (2017)

3. **Assessing the distinguishable cluster approximation based on the triple bond-breaking in the Nitrogen molecule**. Varun Rishi, Ajith Perera and Rodney J. Bartlett. J. Chem. Phys. 144, 124117 (2016)

2. **Approximating electronically excited states with equation-of-motion linear coupled cluster theory**. Jason Byrd, Varun Rishi, Ajith Perera and Rodney J. Bartlett. J. Chem. Phys. 143, 164103 (2015)

1. **Transition metal atomic multiplet states through the lens of single reference coupled-cluster and the equation-of-motion coupled-cluster methods**. Varun Rishi, Ajith Perera and Rodney J. Bartlett. Theor. Chem. Acc. 133, 1515 (2014)

Talks

Invited

12. **Predicting Photochemistry with Novel Quantum Methods**, University of Calgary, Alberta, Canada (Nov 2023)

11. **Dark Doubly Excited States and Non-adiabatic Mixed Quantum-Classical Dynamics: New Frontiers for Equation-of-motion Coupled Cluster Methods**, Sanibel Symposium, St. Augustine, Florida (Feb 2023)

10. **Opportunities at the Intersection of Quantum Chemistry with High Performance Computing, Machine Learning and Quantum Computing**, *Future of Chemistry* Symposium series, Tata Institute of Fundamental Research, Mumbai (Jan 2022)

9. **Quantum chemistry beyond the usual: Transition metals, doubly excited states and potential energy surfaces**, Sandia National Lab (Aug 2021)

8. **Theoretical tools to design functional molecules**, Indian Institute of Science Education & Research, Thiruvananthapuram (Feb 2021)

7. **Overcoming the cost barrier in quantum chemistry**, Indian Institute of Science Education & Research, Tirupati (Oct 2020)

6. **Treating strong correlation with internally corrected coupled cluster methods: Is distinguishable cluster approach systematically improvable?**, Sanibel Award Lecture, Sanibel Symposium, St. Simons Island, Georgia (Feb 2019)

5. **The search for a coupled cluster method that works in weak and in strong correlation**, Department of Chemistry, Virginia Tech, Virginia (May 2017)

   Contributed

4. **Ultrafast photofragmentation of Dimethyl Disulphide in far-UV light: Elucidating reaction pathways with non-adiabatic mixed quantum-classical (NA-MQC) dynamics**, American Chemical Society (ACS) National meeting in Indianapolis, Indiana (March 2023)

3. **Reducing the scaling of higher-order coupled cluster methods through tensor decomposition techniques** Sanibel Symposium, St. Simons Island, Georgia (Feb 2018)

2. **Excited states from approximate CCSD methods: better than EOM-CCSD?** South Eastern Theoretical Chemist Association (SETCA) meeting at Florida State University, Tallahassee (May 2016)

1. **Approximate Coupled-Cluster methods: a case of addition by subtraction?** American Chemical Society (ACS) National meeting in San Diego, California (March 2016)

Posters

1. **Designing a new class of coupled cluster methods for strong correlation with reduction in scaling via tensor decomposition**. Varun Rishi, Karl Pierce and Edward F. Valeev. 9th Molecular Quantum Mechanics Conference, Heidelberg (2019)

2. **The Reach and Limits of a *Double Excitations Only* Model in Coupled Cluster Theory**. Varun Rishi and Rodney J. Bartlett. Sanibel Symposium, St. Simons Island (2017)

3. **Improving upon approximate CCSD methods: how to add the effect of higher excitations**. Varun Rishi, Ajith Perera and Rodney J. Bartlett. Theory and Applications of Computational Chemistry (TACC), Seattle (2016)

4. **Ab-initio Potential energy surfaces for bond dissociation through Coupled-Cluster methods: the case of triple bond-dissociation in nitrogen molecule**. Varun Rishi, Ajith Perera and Rodney J. Bartlett. American Chemical Society National Meeting, San Diego (2016)

5. **Breaking bonds with approximate coupled-cluster methods**. Varun Rishi, Ajith Perera and Rodney J. Bartlett. Sanibel Symposium, St. Simons Island (2016)

6. **Ab-initio study of low-lying spin states of thiolate model of cytochrome p450 Compound I**. Varun Rishi, Jason Byrd, Victor Lotrich and Rodney J. Bartlett. Sanibel Symposium, St. Simons Island (2015)

7. **First Series Transition Metal Multiplets**. Varun Rishi and Rodney J. Bartlett. Sanibel Symposium, St. Simons Island (2013)

Tutorials

- **Modelling chemical reactions on a quantum computer**
  `https://pennylane.ai/qml/demos/tutorial_chemical_reactions`

Teaching

- **University of Florida** Gainesville, USA
  Teaching Assistant, Department of Chemistry *2011 - 2015*
  Prof. James Horvath
  - Introduced the chemistry and pre-medical undergraduates to general chemistry laboratory courses
  - Demonstration and Instructional assistance in performing of experiments
  - Grading of laboratory work, quizzes, unknown samples, and final written exams

Awards & Honours

Sanibel Prize 2018
Recognition for PhD thesis from Quantum Theory Project (QTP) at UF

Outstanding 1st year Physical Chemist 2012
Recognition for academic excellence from division of Physical Chemistry at UF

Graduate Student Fellowship 2011-2015
Recognition of academic excellence amongst incoming graduate students by UF chemistry

'Project Oriented Chemical Education' Fellow at JNCASR, Bangalore, India 2007-2009
A 3 year summer classroom and research training program

GOI Fellowship for Undergraduates in Basic Sciences 2006-2011
Fellowship by Ministry of Human Resource & Development, Government of India

Travel Grants

1. Award by the MolSSI (Molecular Sciences Software Institute) to attend Stochastic Methods School, University of Pittsburg, Pittsburg, Pennsylvania (2019)
2. Award by the MolSSI(Molecular Sciences Software Institute) to attend Summer School and Workshop on Parallel Computing in molecular Sciences, Lawrence Berkeley National lab, Berkeley, California (2018)

3. Award by the Chemical Physics Center at the University of Florida to attend TACC (Theory and applications of computational chemistry), Seattle (2016)
4. Award by Office of Research, University of Florida to attend TACC, Seattle (2016)
5. Award by Office of Research, University of Florida to attend ACS National meeting in San Diego (2016)

Service and Outreach

- Reviewer for American Institute of Physics (AIP) journals *Journal of Chemical Physics* and *Journal of Applied Physics*
- Reviewer for American Chemical Society (ACS) journal *Journal of Chemical Theory & Computation*
- Reviewer for Royal Society of Chemistry (RSC) journals *Physical Chemistry Chemical Physics* and *Digital Discovery*
- Member of Editorial Board of *Frontiers in Chemistry* journal
- Chair of poster session at the Sanibel Symposium on Theoretical Chemistry (2016), St. Simons Island, GA
- 'Champions of Change' Award by University of Florida for a sports and socializing initiative for graduate students under the aegis of Corry Cricket Club

References

Prof. Rodney Bartlett **bartlett@qtp.ufl.edu**
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Prof. Edward Valeev **evaleev@vt.edu**
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Virginia Tech, Blacksburg, VA

Dr. Laura McCaslin **lmmccas@sandia.gov**
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