Varun Rishi

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Work Experience

- **Sandia National Labs** — Livermore, USA
  Postdoc, Dr. Laura McCaslin, Combustion Research Facility — *2022 -*
  - Ultrafast chemistry of small organic molecules probed by theoretical and experimental spectroscopy
- **Xanadu Quantum Technologies Inc.** — Toronto, Canada
  Independent Contractor(Quantum Algorithms) — *2021*
  - Devising algorithms to simulate chemical systems on near-term quantum computers
- **California Institute of Technology** — Pasadena, USA
  Postdoc, Prof. Thomas Miller, Chemistry & Chemical Engineering — *2019 - 2020*
  - Machine Learning the electron correlation problem to predict properties of molecular systems
- **Virginia Tech** — Blacksburg, USA
  Postdoc, Prof. Edward Valeev, Chemistry — *2017 - 2019*
  - Tensor Decomposition techniques for reduced-scaling methods
  - Massively parallel implementation of high-level coupled cluster methods

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*
  - Treatment of strong correlation through coupled cluster methods
  - Development of methods to predict excitation energies and ionization energies
- **Indian Institute of Science Education and Research** — Pune, India
  BS-MS — *2006 - 2011*

  Thesis: *Ab initio quantum chemical study of selenium dioxide mediated allylic hydroxylation of alkenes*
  Supervised by Dr. Sudip Roy, National Chemical Laboratory, Pune

Publications

1. **Varun Rishi**, Moneesha Ravi, Ajith Perera and Rodney J. Bartlett, "Dark Doubly Excited States with Modified Coupled Cluster Models: A Reliable Compromise between Cost and Accuracy?". J. Phys. Chem. A, 127, 828 (2023) https://doi.org/10.1021/acs.jpca.2c07697

2. Karl Pierce, **Varun Rishi** and Edward F.Valeev, "Robust approximation of tensor networks: application to grid-free tensor factorization of the Coulomb interaction". J. Chem. Theory Comput. 17, 4, 2217 (2021) https://doi.org/10.1021/acs.jctc.0c01310

3. Justus Calvin, Chong Peng, **Varun Rishi**, Ashutosh Kumar and Edward F. Valeev, "Many-body quantum chemistry on massively parallel computers". Chem. Rev. 121, 3, 1203 (2021) https://doi.org/10.1021/acs.chemrev.0c00006

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

5. Chong Peng, Cannada A. Lewis, Xiao Wang, Marjory C. Clement, Karl Pierce, **Varun Rishi**, Fabijan Pavošević, Samuel Slattery, Jinmei Zhang, Nakul Teke, Ashutosh Kumar, Conner Masteran, Andrey Asadchev, Justus A. Calvin and Edward F. Valeev,"Massively Parallel Quantum Chemistry : A High-Performance Research Platform for Electronic Structure". J. Chem. Phys. 153, 044120 (2020)

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

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

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

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

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

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

Preprint

- **Varun Rishi**, Neil Cole-Filipiak, Krupa Ramasesha and Laura M. McCaslin, "Unveiling the UV photofragmentation pathways of dimethyl disulfide initiated by a Rydberg excitation" ChemRxiv (2023) https://doi.org/10.26434/chemrxiv-2023-bnj1b

Talks

Invited

1. "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)

2. "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)

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

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

5. "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)

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

Contributed

1. "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)

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

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

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

Posters

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

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

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

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

5. **Varun Rishi**, Ajith Perera and Rodney J. Bartlett, "Breaking bonds with approximate coupled-cluster methods", Sanibel Symposium, St. Simons Island, Georgia, USA (2016)
6. **Varun Rishi**, Jason Byrd, Victor Lotrich and Rodney J. Bartlett, "Ab-initio study of low-lying spin states of thiolate model of cytochrome p450 Compound I", Sanibel Symposium, St. Simons Island, Georgia, USA (2015)
7. **Varun Rishi** and Rodney J. Bartlett, "First Series Transition Metal Multiplets", Sanibel Symposium, St. Simons Island, Georgia, USA (2013)

Research Grants

- Lead Principal Investigator for LDRD (Laboratory Directed Research & Development) grant by Sandia National Lab titled "Towards efficient light emitters via computational design of molecules with inverted singlet-triplet gaps" ($43000) (2023)

Software

- The Massively Parallel Quantum Chemistry Program (MPQC), Version 4.0.0-beta.1
  Chong Peng, Cannada Lewis, Xiao Wang, Marjory Clement, Fabijan Pavosevic, Jinmei Zhang, **Varun Rishi**, Nakul Teke, Karl Pierce, Justus Calvin, Joseph Kenny, Edward Seidl, Curtis Janssen and Edward Valeev.

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

POCE fellowship 2007-2009
'Project Oriented Chemical Education' fellow at JNCASR, Bangalore, India
A 3 year summer classroom and research training program leading to a degree of Diploma in Chemistry

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

- Member of Editorial Board of *Frontiers in Chemistry* journal
- Reviewer for Royal Society of Chemistry (RSC) journals *Physical Chemistry Chemical Physics* and *Digital Discovery*
- Chaired a 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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University of Florida, Gainesville, FL

Prof. Edward Valeev **evaleev@vt.edu**
Department of Chemistry Phone: 1-540-231-8218
Virginia Tech, Blacksburg, VA

Dr. Laura McCaslin **lmmccas@sandia.gov**
Sandia National Laboratories Combustion Research Facility Phone: 1-925-294-3439
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