Ayush Asthana

Current Position:	Postdoctoral Research Associate in Quantum Computing
University:	Virginia polytechnic institute and state university
Contact:	ayushasthana15@gmail.com, +1 443-708-6400
LinkedIn Profile:	linkedin.com/in/ayushasthana
GitHub Profile:	github.com/aasthan4
Personal website:	aasthan4.github.io/
Research Interest:	Quantum Computing, Quantum Chemistry, Scientific Computing

Employment

Aug 2021-current **Postdoctoral Research Associate, Virginia Tech**
Advisor: Prof. Nicholas J. Mayhall
Project 1: Pulse-level variational molecular simulation
Project 2: Development of molecular excited state methods for NISQ era devices

May 2014-July 2014 **Undergraduate Summer Research Intern**
Advisor: Prof. T. Daniel Crawford
Computational study of optical rotation in small molecules and theoretical chemistry summer school

Education

2016-2021 **PhD in Theoretical Chemistry, Johns Hopkins University**
Advisor: Prof. Lan Cheng
Dissertation: Development of relativistic quantum chemistry methods for heavy-element containing molecules

2011-2016 **BS-MS Dual Degree in Chemistry, Indian Institute of Technology Kanpur**
Advisors: Prof. Debashis Mukherjee (IACS), co-advisor: Prof. Srihari Keshavamurthy (IITK)
Thesis: Treatment of Bond Breaking and handling of Quasi-Degeneracy: Formulation of a multi-reference analog of Single reference Perturbation Theory of 2nd order

Certifications

July 2020 Global Summer School on Quantum Computing by IBM (Certificate)
May 2020 Professional certificate in Quantum Computing and Quantum Internet
Delft University of Technology in collaboration with edX

Publications

1. **A. Asthana** A. Kumar, V. Abraham, H. Grimsley, Y. Zhang, L. Cincio, S. Tretiak, P. Dub, S. Economou, E. Barnes, N. Mayhall, "Equation-of-motion variational quantum eigensolver method for computing molecular excitation energies, ionization potentials, and electron affinities", arxiv.org/abs/2206.10502 (2022).
2. **A. Asthana**, C. Liu, O. R. Meitei, S. E. Economou, E. Barnes, N. J. Mayhall, "Minimizing state preparation times in pulse-level variational molecular simulations", arxiv.org/abs/2203.06818 (2022).
3. A. Kumar, **A. Asthana**, C. Masteran, E. F. Valeev, Y. Zhang, L. Cincio, S. Tretiak, P. A. Dub, "Accurate quantum simulation of molecular ground and excited states with a transcorrelated Hamiltonian", arxiv.org/abs/2201.09852 (2022).
4. J. Liu, X. Zheng, **A. Asthana**, C. Zhang, and L. Cheng, "Analytic Evaluation of Energy First Derivatives for Spin-Orbit Coupled-Cluster Singles and Doubles Augmented with Noniterative Triples Method: General Formulation and An Implementation for First-Order Properties", J. Chem. Phys. **154**, 064110 (2021).
5. G. Liu, C. Zhang, S. Ciborowski, **A. Asthana**, L. Cheng and K. Bowen, "Mapping the Electronic Structure of the Uranium (VI) Dinitride Molecule, UN_2", J. Phys. Chem. A, **124**, 6486 (2020).
6. **A. Asthana**, J. Liu, and L. Cheng, "Exact two-component equation-of-motion coupled-cluster singles and doubles method using atomic mean-field spin-orbit integrals", J. Chem. Phys. **150**, 074102 (2019).
7. J. Liu, **A. Asthana**, L. Cheng, and D. Mukherjee, "Unitary coupled-cluster based self-consistent polarization propagator theory: A third-order formulation and pilot applications"J. Chem. Phys. **148**, 244110 (2018).
8. J. Liu, Y. Shen, **A. Asthana**, and L. Cheng, "Two-component relativistic coupled-cluster methods using mean-field spin-orbit integrals", J. Chem. Phys. **148**, 034106 (2018).

Presentations

Invited

- Relativistic coupled-cluster methods for heavy-element computational chemistry (Invited talk). IBM Almaden Research Center, Jul 2020

Other

- Equation-of-motion variational quantum eigensolver method for computing molecular excitation energies, ionization potentials, and electron affinities (Oral presentation). American Chemical Society National Meeting Chicago, IL August 2022
- Minimizing pulse level variational molecular simulation (Oral presentation). American Chemical Society National Meeting Chicago, IL August 2022
- Equation-of-motion variational quantum eigensolver method for computing molecular excitation energies, ionization potentials, and electron affinities (Poster presentation). Molecular Quantum Mechanics (MQM), Blacksburg, June 2022
- Pulse-level variational molecular simulation (Oral presentation). Quantum Information Science symposium at Virginia Tech, April 2022
- Minimizing state preparation times in pulse-level variational molecular simulation (Oral presentation). American Physical Society National Meeting Chicago, IL March 2022
- New algorithmic development for relativistic equation-of-motion coupled-cluster method (Poster presentation). American Chemical Society National Meeting & Exposition, San Francisco, CA, Aug 2020
- Development of relativistic quantum chemistry methods for molecules containing heavy-elements (Graduate Board Oral talk). Johns Hopkins University, Dec 2019
- Chemistry at ultracold temperatures (Department seminar). Johns Hopkins University, Mar 2019
- Extended wick's theorem, spin free cumulants and their role in formulation and analyzing spacial and spin correlation of many electron systems (Master's thesis talk). Indian Institute of Technology Kanpur, Apr 2016

Organized symposium

- Co-organizer of Virginia Tech Quantum (VTQ) symposium, a two day symposium with more than 40 participants from the department of Physics, Computer Science and Chemistry, April 2022

Achievements and Scholarships

May 2016	Recepient of best master's project award, Department of Chemistry, IIT Kanpur.
2011-2016	Awarded *INSPIRE-SHE Scholarship* worth $6000, Department of Science and Technology, Government of India.
May 2011	Secured a position in the top 1% All India Rank in IIT-JEE 2011 competitive exam with more than 500,000 participants.
May 2011	Secured a top 0.2% All India Rank in AIEEE 2011 and UPTU 2011 competitive exams with over 1.1 million and 0.5 million participants, respectively.

Research Experience

Pulse-level variational molecular simulation

2021-present, Mayhall Lab, *Postdoctoral research associate, Virginia Tech, USA*

- Develop algorithms and code for simulation of pulse-level VQE algorithm for the calculation of molecular ground states.
- Apply ideas from quantum control theory and variational quantum eigensolver algorithms to understand fundamental aspect of computation on a quantum computer.
- Collaborate with theoretical and experimental teams to implement pulse-level VQE.

Relativistic spin-orbit coupled-cluster methods for heavy-element computational chemistry

2016-2021, Cheng Lab, *Graduate Research Assistant, Johns Hopkins University, USA*

- Developed efficient implementation of spin-orbit coupled-cluster (SO-CC) methods to treat relativistic effects in compounds containing heavy-elements.
- Developed atomic-orbital (AO) based algorithms, using spin-symmetry and sparsity in AO two-electron integrals, to reduce computational requirements in SO-CC methods.
- Developed efficiently parallelized code using shared-memory intranode (OpenMP) parallelization strategy, along with load-balancing algorithms.

Automatic expression generator, application to unitary coupled-cluster based methods Git:git/autogen

2016-present, Cheng Lab, *Graduate Research Assistant, Johns Hopkins University, USA*

- Develop a python based open-source automatic expression generator for electronic structure theories, capable of deriving hundreds of working expressions in the form of tensor contractions.
- Derive working expressions for unitary coupled-cluster theory based methods.

Treatment of Bond Breaking and handling of Quasi-Degeneracy: Formulation of a multi-reference analog of Single reference Perturbation Theory of 2nd order

Jan-Apr 2016, Mukherjee Lab, *Master's Thesis Researcher, Indian Association for Cultivation of Sciences, India*

- Developed formalism for a multi-reference analog of single-reference perturbation theory of second order.
- Developed code for spin-free generalized wick's theorem that allows to implement the formalism.
- Analysed the behavior of spin-free cumulants through $CH4^{+}$ molecule undergoing dissociation.

Computational study for Optical Rotation of molecules
May-Jul 2014, Crawford lab, *Summer Research Fellow, Virginia Tech, USA*

- Investigated the relationship of excited state contributions to the optical rotation with the changes in dihedral angle for several molecules.
- Developed pilot programs for doing Hartree-Fock (HF) and post-HF calculations on small molecule test cases.

Technical Skills

Programming:	FORTRAN including packages like LAPACK,Python including packages like NumPy,C, C++,Q#,Qiskit
Applications:	CFOUR, Gaussian, PSI4, PySCF, GaussView, Gnuplot, gmol
	Experienced in parallel programming using OpenMP and MPI
Methods:	Expert level knowledge in electronic structure theory such as CC and DFT.
Misc:	LaTeX, Linux, Mathematica, Git

Software Contributions

AutoGen	- Developed open-sourced python-based automatic expression generator package for quantum chemical theories. - The program used wick's theorem to automatically derive working expressions. Deriving hundreds of these expressions, as in the case of unitary coupled-cluster (UCC) theory, can be time-taking and error-prone when done by hand.
CFOUR	- Contributor in CFOUR (Coupled-Cluster techniques for Computational Chemistry) chemistry program, an international collaborative program for high accuracy molecular calculations. - Contributed an efficient implementation of relativistic spin-orbit coupled-cluster methods for calculations of molecules containing heavy-elements.