Ayush Asthana

Current Position:	Postdoctoral Research Associate in Quantum Computing
Department, University:	Department of Chemistry, Virginia Tech
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Research Interest:	Quantum Information Science, Quantum Control, Quantum Chemistry

Employment

Aug 2021-current — **Postdoctoral Research Associate, Virginia Tech**
Advisor: Prof. Nicholas J. Mayhall
- Quantum computing using principles of quantum control theory
- Quantum chemistry on near-term quantum computers

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

Education

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

Jul 2011- May 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

Jul 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

Pre-publications (Submitted for Peer-review)

*- corresponding author

1. A. Kumar*, **A. Asthana**, V. Abraham, T. Crawford, N. Mayhall, Y. Zhang, L. Cincio, S. Tretiak, P. Dub*, "Quantum simulation of molecular response properties", arxiv.org/abs/2301.06260 (Submitted to Chemical Science, RSC) (2022).
2. **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 (Minor revisions at Chemical Science, RSC) (2022).
3. **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 (under review at Physical Review X) (2022).

Publications (Peer-reviewed)

4. 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", J. Chem. Theory Comput. **18**, 9, 5312 (2022).
5. 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).
6. 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).
7. **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).
8. 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).

9. 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

1. Path to quantum chemistry on near-term quantum computers, VTQ internal seminar, Virginia Tech, Dec 2022
2. Pulse-level molecular simulation on transmon qubits. Applied Physics Lab, Johns Hopkins University, Nov 2022
3. Towards quantum chemistry on near-term quantum computers, Quantinuum (Honeywell), UK, Oct 2022
4. Pulse-level variational molecular simulation. Oak Ridge National Lab, Jul 2022
5. Relativistic coupled-cluster methods for heavy-element containing molecules. Virginia Tech, Mar 2021
6. Relativistic quantum chemistry methods for heavy-element computational chemistry. IBM Almaden Research Center, Jul 2020

Contributed

7. Role of orbital-optimization molecular ground and excited-state calculations on quantum computer (Oral presentation). American Physical Society National Meeting Las Vegas, NV Mar 2023
8. 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 Aug 2022
9. Minimizing pulse level variational molecular simulation (Oral presentation). American Chemical Society National Meeting Chicago, IL Aug 2022
10. Equation-of-motion variational quantum eigensolver method for computing molecular excitation energies, ionization potentials, and electron affinities (Poster presentation). Molecular Quantum Mechanics (MQM), Blacksburg, Jun 2022
11. Pulse-level variational molecular simulation (Oral presentation). Quantum Information Science symposium at Virginia Tech, Apr 2022
12. Minimizing state preparation times in pulse-level variational molecular simulation (Oral presentation). American Physical Society National Meeting Chicago, IL Mar 2022
13. New algorithmic development for relativistic equation-of-motion coupled-cluster method (Poster presentation). American Chemical Society National Meeting & Exposition, San Francisco, CA, Aug 2020
14. Development of relativistic quantum chemistry methods for molecules containing heavy-elements (Graduate Board Oral talk). Johns Hopkins University, Dec 2019
15. Chemistry at ultracold temperatures (Department seminar). Johns Hopkins University, Mar 2019
16. Extended wick's theorem, spin-free cumulants and their role in the formulation and analyzing spacial and spin correlation of many-electron systems (Master's thesis talk). Indian Institute of Technology Kanpur, Apr 2016

by collaborators

- Zhao T. et. al., Gate-free VQE Exploiting Inter-qubit Parametric Interaction (Oral presentation). American Physical Society National Meeting Las Vegas, NV Mar 2023
- Kumar A. et. al., Accurate quantum chemistry calculations using NISQ era quantum computers (Oral presentation). American Physical Society National Meeting Las Vegas, NV Mar 2023
- Liu C. et. al., Implementing pulse-based VQE (ctrl-VQE) algorithm on NISQ devices. (Oral presentation). American Physical Society National Meeting Las Vegas, NV Mar 2023

Organized

- Co-organizer of Virginia Tech Quantum (VTQ) seminar series, Jan-May 2023
- 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 Services

Dec 2022	Committee member for masters thesis defence of a visiting student at Virginia Tech in Crawford lab.
2020 to 2022	Reviewer in Chemical Science (RSC), Journal of chemical theory and computation (ACS), ACS Central Science.
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.

Software Contributions

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.
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.
Adapt-vqe	- Contributed methods for molecular excited-state energy (QSE, qEOM and q-sc-EOM) using simulations of adapt-VQE algorithm for ground-state wavefunction. - Resulted in two scientific publications (submitted).