Ayush Asthana

Current Position:	Assistant Professor
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Group website:	theasthanagroup.com
Research Interest:	Quantum Chemistry, Quantum Computing, Quantum Control

Employment

Aug 2023-current	**Assistant Professor of Chemistry (Tenure Track)** and **Adjunct Professor of Physics** University of North Dakota - quantum chemistry and quantum computing
Aug 2021-Jul 2023	**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

Pre-publications (Submitted for Peer-review)

1. P. F. Kwao, S. P. Sundar, B. Gupt and **A. Asthana**, "On the generalized eigenvalue problem in subspace-based excited state methods for quantum computers", arxiv.org/2503.09670 (2015).

Publications (Peer-reviewed)

2. C. Zhang, X. Zheng, J. Liu, **A. Asthana**, and L. Cheng*, "Analytic gradients for relativistic exact-two-component equation-of-motion coupled-cluster singles and doubles method", J. Chem. Phys. **159**, 244113 (2023).
3. A. Kumar*, **A. Asthana**, V. Abraham, T. Crawford, N. Mayhall, Y. Zhang, L. Cincio, S. Tretiak, P. Dub*, "Quantum simulation of molecular response properties", J. Chem. Theory Comput. **19**, 24, 9136 (2023) .
4. **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", Phys. Rev. Applied **19**, 064071, (2023).
5. **A. Asthana*** A. Kumar, V. Abraham, H. Grimsley, Y. Zhang, L. Cincio, S. Tretiak, P. Dub, S. Economou, E. Barnes, N. Mayhall*, "quantum self-consistent equation-of-motion method for computing molecular excitation energies, ionization potentials, and electron affinities", Chem. Sci., **14**, 2405 (2023).
6. 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).
7. 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).
8. 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).
9. **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).
10. 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).

11. 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).

GRANTS

Aug 2024	Grant from a leading pharma company, Moderna Inc. to investigate "Accurate and Scalable molecular simulations on quantum computers" (role: PI, total amount: $24,600 with $24,600 for Asthana Lab for 6 months).
Sept 2024	**NSF Epscor Research Fellow:** "Quantum Algorithms for Early Fault-tolerant Quantum Computers" (role: PI, total amount: $300,000 with $300,000 for Asthana Lab).
Aug 2024	**NSF Expand QISE:** "Quantum Algorithms for Relativistic Quantum Chemistry" (role: PI, total amount: $800,000 with $560,000 for Asthana Lab).
Nov 2023	Early Career Scholars Program to Advance Multi-Disciplinary Research Teams - UND internal funding award (role: PI, amount: $30,000 with $15,000 for Asthana Lab).
Nov 2023	$5000 Compute credits from Amazon Braket

Presentations

Invited

1. The University of Minnesota April 2025, Upcoming.
2. The University of Rhode Island Nov 2024, "Towards quantum chemistry using quantum computers" webpage.
3. (Keynote talk) IEEE 2024 workshop in Chemical Applications of Quantum Computing, Montreal, Canada, "Towards simulating molecular excited states on quantum computers" Sept 2024 webpage.
4. Concordia University Mar 2024, "Quantum chemistry on quantum computers".
5. Questaal Workshop in NREL, Mar 2024, "Quantum chemistry in the era of quantum computing - opportunities and challenges", webpage.
6. American Physical Society National Meeting Minneapolis, MN Mar 2024, "Towards simulating molecular excited states on quantum computers", web.
7. TIFR Mumbai, Dec 2023, "Quantum chemistry in the era of quantum computing - opportunities and challenges".
8. IIT Bombay, Dec 2023, "Quantum chemistry in the era of quantum computing - opportunities and challenges".
9. University of Hyderabad, Nov 2023, "Quantum chemistry in the era of quantum computing - opportunities and challenges".
10. Pacific Northwest National Lab, Nov 2023, "Quantum chemistry in the era of quantum computing, opportunities and challenges".
11. University of North Dakota Physics, Oct 2023,"Towards molecular simulation on quantum computers".
12. (Keynote talk) IEEE Quantum Week, Workshop on Quantum Computing for Natural Sciences: Technology and Applications Sept 2023, "Molecular excited states on quantum computers".
13. University of North Dakota, (Job talk) Apr 2023, "Towards molecular simulation on quantum computers".
14. Quantum Brilliance, Germany, Feb 2023, "Towards molecular simulation on near-term quantum computers".
15. VTQ symposium, Virginia Tech, Feb 2023 "Pulse-level molecular simulation algorithms for near-term quantum computers".
16. VTQ internal seminar, Virginia Tech, Dec 2022, "Path to quantum chemistry on near-term quantum computers".
17. Applied Physics Lab, Johns Hopkins University, Nov 2022, "Pulse-level molecular simulation on transmon qubits".
18. Quantinuum (Honeywell), UK, Oct 2022, "Towards quantum chemistry on near-term quantum computers".
19. Oak Ridge National Lab, Jul 2022, "Pulse-level variational molecular simulation".
20. Virginia Tech, Mar 2021, "Relativistic coupled-cluster methods for heavy-element-containing molecules".
21. IBM Almaden Research Center, Jul 2020, "Relativistic quantum chemistry methods for heavy-element computational chemistry".

Contributed

22. APS march meeting March 2025, "Advances in molecular excited state methods for quantum computers."
23. Midwest Theoretical Chemistry Conference, Purdue U, IN Jun 2023, "New method for excited-state calculations on near-term quantum computer.

24. American Physical Society National Meeting Las Vegas, NV Mar 2023, "Role of orbital-optimization molecular ground and excited-state calculations on quantum computer (Oral presentation)".
25. American Chemical Society National Meeting Chicago, IL Aug 2022, "Equation-of-motion variational quantum eigensolver method for computing molecular excitation energies, ionization potentials, and electron affinities (Oral presentation)".
26. American Chemical Society National Meeting Chicago, IL Aug 2022, "Minimizing pulse level variational molecular simulation (Oral presentation)".
27. Molecular Quantum Mechanics (MQM), Blacksburg, Jun 2022, "Equation-of-motion variational quantum eigensolver method for computing molecular excitation energies, ionization potentials, and electron affinities (Poster presentation)".
28. Quantum Information Science symposium at Virginia Tech, Apr 2022, "Pulse-level variational molecular simulation (Oral presentation)".
29. American Physical Society National Meeting Chicago, IL Mar 2022, "Minimizing state preparation times in pulse-level variational molecular simulation (Oral presentation)".
30. American Chemical Society National Meeting & Exposition, San Francisco, CA, Aug 2020, "New algorithmic development for relativistic equation-of-motion coupled-cluster method (Poster presentation)".
31. Johns Hopkins University, Dec 2019, "Development of relativistic quantum chemistry methods for molecules containing heavy-elements (Graduate Board Oral talk)".
32. Johns Hopkins University, Mar 2019, "Chemistry at ultracold temperatures (Department seminar)".
33. Indian Institute of Technology Kanpur, Apr 2016, "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)".

Media

- UND: NSF award news
- Quantum researchers collide, Virginia Tech, Exponentially More

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.

Teaching

Spring 2024	Quantum Mechanics in Chemistry (Review 4.7/5)
Fall 2024	(Newly developed) Applied Quantum Computing

Mentoring

Postdocs	Dr. Srivathsan Poyyapakkam Sundar (since Aug 2024)
Graduate students	Prince Fredrick Kwao (second year)
Undergraduate students	Sean Glaholt (co-advised by Prof. Yen Lee Loh - Physics)

Services

Nov 2024	NSF review panel member(2024)
June 2024-current	Guest editor in Quantum Science and Technology, IOP focus issue on quantum computing applications in chemistry.
2023 to current	Member of the editorial board for the Quantum Computing paper track for ISC High Performance 2024.
Jan-May 2023	Co-organized Virginia Tech Quantum (VTQ) seminar series
2020 to current	Reviewer in NPJ Quantum Information (Nature), Chemical Science (RSC), Journal of Chemical Theory and computation (ACS), ACS Central Science, Journal of Chemical Physics (AIP).
April 2022	Co-organized Virginia Tech Quantum (VTQ) symposium, a two-day symposium with more than 40 participants from the Department of Physics, Computer Science and Chemistry

Achievements

Dec 2024	UND early career scholar award.
Nov 2024	NSF Epscor research fellow award.
May 2016	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.