Ayush Asthana

Current Position:	Senior Ph.D. researcher in Quantum Chemistry
University:	Johns Hopkins University
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Research Interest:	Quantum Chemistry, Quantum Computing, Scientific Computing

Professional summary

- Theoretical scientist working in the development of quantum chemistry methods for electronic structure calculations for heavy element chemistry.
- 5+ years of research experience in developing quantum chemical methods for high-accuracy electronic structure calculations in chemistry.
- 7+ years of experience in developing production level code in science and contributing to open-source software in FORTRAN and Python coding languages; including implementation for large high-performance computers using OpenMP and MPI.

Education

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

2011-2016 **BS-MS Dual Degree in Chemistry, Indian Institute of Technology Kanpur** (GPA: 8.2/10)
Advisors: Prof. Debashis Mukherjee (IACS) and 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

Technical Skills

Languages:	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:	Strong theoretical and computational understanding in electronic structure theory such as CC and DFT
Misc:	LaTeX, Linux, Mathematica, Git

Certifications

May 2020 Professional certificate in Quantum Computing and Quantum Internet
Delft University of Technology in collaboration with edX

July 2020 Global Summer School on Quantum Computing by IBM (Certificate)

Achievements and Scholarships

2016-present Awarded fellowship by the Department of Chemistry at JHU to carry out research in quantum chemistry, worth $85,000 per year.

May 2016 Awarded best Master's project award by the Department of Chemistry, IIT Kanpur.

2011-2016 Awarded *INSPIRE-SHE Scholarship* by the Department of Science and Technology, Government of India worth $6000.

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 Projects

AutoGen

- Developed open-sourced python based automatic expression generator package for quantum chemical theories.
- Used wick's theorem to automatically derive working equations to be coded. Deriving hundreds of these equations is time taking and error-prone if done by hand.
- Slashed working-equation derivation time for quantum chemical theories by months and eliminated chances of human error.
- Established collaboration in the development of unitary coupled-cluster theory at Department of Chemistry, JHU which resulted in 1 co-authored publication in a peer-review journal and 1 manuscript under preparation.

CFOUR

- Contributor in CFOUR (Coupled-Cluster techniques for Computational Chemistry) chemistry program, an international collaborative program for high accuracy molecular calculations.
- Contributed an efficient atomic-orbital based implementation of relativistic coupled-cluster methods for calculations of molecules containing heavy elements.
- Notable algorithmemic solutions include design of a sparse-dense type tensor-tensor contraction for large tensor contractions, efficiently parallelized by improved load-balancing among processors.

Research Experience

Relativistic coupled-cluster methods for heavy-element computational chemistry

Graduate Research Assistant, Johns Hopkins University, USA 2017-present

- Developing efficient implementation of spin-orbit coupled-cluster methods to treat relativistic effects in compounds containing heavy elements.
- Used efficient parallelization techniques and developed atomic-orbital based algorithms to reduce storage requirements by an order of magnitude and speed-up the calculation making use of tens of processors.
- Collaborated with experiment lab at JHU to compare experimental excitation energies with theoretical calculations for UN_2 molecule.
- Contributed in DOE sponsored project with 3 co-authored papers so far.

Unitary coupled-cluster theory development through automatic expression generation, Git:git/autogen

Graduate Research Assistant, Johns Hopkins University, USA 2017-present

- Collaborating in the development of unitary coupled-cluster theory based methods.
- Developed a python based open-source automatic expression generator for electronic structure theories which can derive working expressions for various formalism of unitary coupled-cluster theory, assisting in the development.
- Developed a collaboration which has reduced derivation time for working equations from months to seconds, eliminated human error and resulted in 1 co-authored publication.

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

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

- Developed formalism for multi-reference analog of single reference perturbation theory of second order.
- Developed the program for spin-free extended wick's theorem based derivation of expressions for the theory.

Computational study for Optical Rotation of molecules

Summer Research Fellow, Virginia Tech, USA May-Jul 2014

- Investigated the relationship of excited states contribution to Optical Rotation with the changes in dihedral angle was studies for simple molecules.
- Developed pilot programs for doing Hartree-Fock (HF) and post-HF calculations on small molecules.

Kinetic Monte Carlo simulation model for Ge on Si surfaces

Undergraduate Research Fellow, IIT Kanpur, India May 2013-Apr 2014

- Developed Kinetic Monte Carlo based solid on solid models to simulate the surface properties of Ge on Si semiconductors.

-Special features were the use of highly optimized 2600 class rejection free kinetic Monte Carlo algorithm and a depth-first search based algorithm for data analysis.

Publications

1. 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", (submitted in J. Chem. Phys. 2020).
2. 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", (submitted in J. Phys. Chem. Lett. 2020).

3. **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).
4. 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).
5. 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

- 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

Relevant Courses

Physical Chemistry:	Electronic Structure Theory, Molecule Radiation Interaction, Molecular Spectroscopy, Statistical Mechanics and its application to Chemistry, Quantum Mechanics, Molecular Modelling, Group Theory.
Computer Science:	Parallel Programming, Data structures and Algorithms, Programming in Chemistry, Fundamentals of Computing.
Quantum Computing:	Architecture, Algorithms, and Protocols of a Quantum Computer and Quantum Internet (MOOC), The Hardware of a Quantum Computer (MOOC).

Other Projects

Parallel implementation and analysis of a new lowest eigenvalue finding algorithm for potential applications in Quantum Chemistry (Report)

> *Course: Parallel Programming, Mentor: Prof. Randal Burns*, Spring, 2016-17
> - Designed the project to implement newly developed algorithm to find the lowest eigenvalue for large matrices.
> - This algorithms has high scalability and potential applications to Quantum Chemistry.
> - Analysed the performance of the algorithm based on OpenMp and MPI based implementation.