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

- Quantum Chemistry researcher working on the development of quantum chemistry methods for electronic structure calculations for heavy element chemistry.
- 5+ years of research experience in developing high-accuracy electronic structure methods in chemistry.
- 7+ years of expertise 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

Programming Languages:	FORTRAN including packages like LAPACK, Python including packages like NumPy, C, C++
Quantum Programming:	Q#, Qiskit
Applications:	CFOUR, Gaussian, PSI4, PySCF, GaussView, Gnuplot, gmol
	Experienced in parallel programming using OpenMP and MPI
Methods:	Strong background 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 worth $85,000 per year, Department of Chemistry at JHU.

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

Relativistic coupled-cluster methods for heavy-element computational chemistry
2017-present, *Graduate Research Assistant, Johns Hopkins University, USA*

- Develop efficient implementation of spin-orbit coupled-cluster methods to treat relativistic effects in compounds containing heavy elements.
- Use 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.
- Collaborate with experiment group at JHU to compare experimental excitation energies with theoretical calculations.
- Contribute in DOE sponsored project with 4 co-authored papers currently.

Unitary coupled-cluster theory development through automatic expression generation, Git:git/autogen
2017-PRESENT, *Graduate Research Assistant, Johns Hopkins University, USA*

- Collaborate in the development of unitary coupled-cluster theory based methods.
- Develop 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.
- The collaboration has reduced derivation time for working equations from months to seconds and eliminated human error.
- This collaboration has also resulted in 1 co-authored publication currently.

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, *Master's Thesis Researcher, Indian Association for Cultivation of Sciences, India*

- 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
MAY-JUL 2014, *Summer Research Fellow, Virginia Tech, USA*

- 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
MAY 2013-APR 2014, *Undergraduate Research Fellow, IIT Kanpur, India*

- 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

Software Projects

AutoGen

- Developed open-sourced python based automatic expression generator package for quantum chemical theories.
- The program used wick's theorem to automatically derive working equations to be coded. Deriving hundreds of these equations, as in the case of unitary coupled-cluster (UCC) theory, is time taking and error-prone if done by hand.
- Established collaboration in the development of UCC theory at Cheng lab, JHU which resulted in 1 co-authored publication in a peer-reviewed journal so far.

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 algorithms based implementation of relativistic spin-orbit coupled-cluster methods for calculations of molecules containing heavy elements.
- The implementation makes use of sparsity in AO integrals and reduces computational requirements by newly implemented sparse-dense type tensor-tensor contractions, efficiently parallelized by load-balancing algorithms.

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.