Ashutosh Kumar – Curriculum Vitae

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Date of Birth	13^{th} September 1989	**Email**	akumar1@lanl.gov
Nationality	Indian		

Education

2013-2018 PhD in theoretical chemistry - Virginia Tech.

Advisor: Dr. T. Daniel Crawford
GPA: 3.83/4.0

2008-2013 Integrated Masters in Chemistry - Indian Institute of Technology, Kharagpur.

Advisor: Dr. P. K. Chattaraj
CGPA: 7.41/10.0

Experience

Jan 2021 - current Los Alamos National Laboratory
Postdoctoral Research Associate: Theoretical division (T-1)

- Working on the extension of the canonical transcorrelated Hamiltonian approach to excited states: this has the potential to drastically reduce the computational resources required for accurate quantum simulations of excited states on NISQ devices. Currently developing an open-source python package to automate the derivation of quantum chemistry expressions required to dress the Hamiltonian.
- Implementing a post-simulation error correction model using reduced-density matrices of correlated many body methods: this is a hybrid model involving both classical and quantum computers where the most computationally expensive parts of the calculations are done on a quantum computer while the classical computer is used to prepare the initial state and correct for the errors produced due to the use of a limited number of qubits.

Aug 2018 - Jan 2021 Virginia Tech
Postdoctoral Research Assistant: Valeev Research Group

- Explicit correlation and Quantum computing: Developed compact Hamiltonians through explicit correlation strategies to increase the accuracy of quantum simulation of electronic structure methods without extra qubits.
- Highly accurate explicit correlation models for large molecular systems: Implemented **DLPNO-CCSD(T)-F12** method in **ORCA 4.2** software package which has enabled accurate energetic studies of open-shell molecules with hundreds of atoms on regular workstations in a few days' time. Working on various optimizations in the codebase to bring down the computational costs even further.
- Massively parallel algorithms for calculating response properties: Implemented distributed memory parallel coupled cluster response models in **MPQC4** software package by leveraging the power of **TiledArray**, a massively parallel block-sparse tensor framework.

Aug 2013 - Jul 2018 Virginia Tech
Graduate Research/Teaching Assistant: Crawford Research Group

- Developed **perturbed-densities** based reduced-scaling approaches which enable significant compression of the wavefunction while maintaining the desired accuracy in calculating coupled cluster linear response properties.
- Contributed to **Psi4** and **Psi4Numpy** open-source quantum chemistry packages: implemented coupled cluster analytic gradients in C++, enabled evaluation of MP2 gradients and hessians in Python through calculations and subsequent export of integral derivatives from C++ to Python, wrote tutorial style codes for calculations of coupled cluster response properties, addressed queries of Psi4 users on the forum, etc.
- Modeled the effects of solute-solvent interactions on chiroptical properties using *frozen-density embedding* models
- Teaching: taught general chemistry lab in 2013; graded and assisted professors in undergraduate courses of PCHEM 1 (Quantum chemistry) and PCHEM 2 (Thermodynamics) in 2014 and 2015.

May 2012 - Jul 2012 Virginia Tech
Short term scholar

- Solvation: Investigated the effects of microsolvation on optical rotation using coupled cluster and density functional theory calculations.
- Programming: Worked on different quantum chemistry programming projects put together by Dr. Daniel Crawford, which focussed on the fundamentals of programming in C/C++ and computer implementations of modern electronic structure theories.

May 2011 - Jul 2011 Kiel University (CAU), Germany
Summer Intern

- Studied non-radiative energy decay mechanisms in enzymes using pump-probe femtosecond laser spectroscopy under Dr. Friedrich Temps; wrote a program in LabView8 to determine the pulse shapes of laser beams.

Awards and Honors

- Published 12 scientific manuscripts in high impact peer-reviewed journals. Has received more than 1100 citations for my research works with a net h-index of 9.
- Reviewer for WIREs Computational Molecular Science scientific journal.
- Best poster award at SETCA conference held at University of Mississippi in May 2017.
- Graduate research award by Department of Chemistry, Virginia Tech for the year 2016-2017.
- Graduate student doctoral award (GSDA) by Graduate School, Virginia Tech for spring semester, 2017.
- Best poster award at 8th MQM Conference held at Uppsala, Sweden in August 2016.
- IAESTE fellowship for research internship at University of Kiel, Germany in 2011.
- INSPIRE scholarship offered by Department of Science and Technology, Govt. of India (2008-2013).

Conferences and Workshops

- Contributed virtual talk at the ACS Conference in Atlanta, Georgia in August 2021.
- Contributed talk at the ACS Conference in San Diego, California in August 2019.
- Contributed talk at the ACS Conference in New Orleans, Louisiana in March 2018.
- Research poster at the WATOC conference, Munich, Germany in August 2017.
- Psi4 developer workshops: University of Georgia (2016), Georgia Tech (2015) and Virginia Tech (2014, 2017).
- Research poster at the 8th Molecular Quantum mechanics conference, Uppsala, Sweden in July 2016.
- Contributed talk at the SETCA conference held at Florida State University, Tallahassee in May 2016.
- Software workshops for Theoretical chemists: Virginia Tech (2015) and Stony Brook University (2014).
- Molecular Response Properties Summer School: Virginia Tech, Blacksburg in July 2015 and June 2017.
- Research posters at the South Eastern Association of Theoretical chemistry (SETCA) conference at Emory University, Atlanta in May 2014 and University of Mississippi, Mississippi in May 2017.

Publications

- **Computing molecular excited states on a D-Wave quantum annealer**, Alexander Teplukhin, Brian K Kendrick, Susan M Mniszewski, Yu Zhang, **Ashutosh Kumar**, Christian FA Negre, Petr M Anisimov, Sergei Tretiak, Pavel A Dub, Scientific reports, 11, 18796 (2021), DOI: https://doi.org/10.1038/s41598-021-98331-y.
- **Explicitly correlated coupled cluster method for accurate treatment of open-shell molecules with hundreds of atoms**, **Ashutosh Kumar**, Frank Neese, and Edward F. Valeev, J. Chem. Phys. 153, 094105 (2020).
- **Quantum simulation of electronic structure with transcorrelated Hamiltonian: improved accuracy with a smaller footprint on the quantum computer**, Mario Motta, Tanvi P. Gujarati, Julia E. Rice, **Ashutosh Kumar**, *et al.*, , Phys. Chem. Chem. Phys., (2020), DOI: 10.1039/D0CP04106H.
- **Many-Body Quantum Chemistry on Massively Parallel Computers**, Justus A. Calvin, Chong Peng, Varun Rishi, **Ashutosh Kumar**, and Edward F. Valeev, Chem. Rev. 2021, 121, 3, 1203–1231.
- **Massively Parallel Quantum Chemistry: A High-Performance Research Platform for Electronic Structure**, Chong Peng, Cannada A. Lewis, Xiao Wang, Marjory C. Clement, Karl Pierce, Varun Rishi, Fabijan Pavošević, Samuel Slattery, Jinmei Zhang, Nakul Teke, **Ashutosh Kumar**, Conner Masteran, Justus A. Calvin, and Edward F. Valeev, J. Chem. Phys. 153, 044120 (2020).
- **Psi4 1.4: Open-source software for high-throughput quantum chemistry**, Daniel Smith, Lori Burns, Andrew Simmonett, Robert Parrish, Matthew Schieber, Raimondas Galvelis, Peter Kraus, Holger Kruse, Roberto Di Remigio, Asem Alenaizan, Andrew James, Susi Lehtola, Jonathon Misiewicz, Maximilian Scheurer, Robert Shaw, Jeffrey Schriber, Yi Xie, Zachary Glick, Dominic Sirianni, Joseph O'Brien, Jonathan Waldrop, **Ashutosh Kumar**, *et al.*, J. Chem. Phys. 152, 184108 (2020).
- **Reduced-scaling coupled cluster response theory: Challenges and opportunities** T. Daniel Crawford, **Ashutosh Kumar**, Alexandre P. Bazanté, Roberto Di Remigio, WIREs Comput Mol Sci 2019;e1406, 1-25 (2019).
- **Psi4NumPy: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development**, Daniel G. A. Smith, Lori A. Burns, Dominic A. Sirianni, Daniel R. Nascimento, **Ashutosh Kumar**, *et al.*, J. Chem. Theory Comp., doi: 10.1021/acs.jctc.8b00286 (2018).

- **Psi4 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability**, Robert M. Parrish, Lori A. Burns, Daniel G. A. Smith, Andrew C. Simmonett, A. Eugene DePrince III, Edward G. Hohenstein, Uighur Bozkaya, Alexander Yu. Sokolov, Roberto Di Remigio, Ryan M. Richard, Jerome F. Gonthier, Andrew M. James, Harley R. McAlexander, **Ashutosh Kumar**, *et al.*, J. Chem. Theory Comp., doi: 10.1021/acs.jctc.7b00174 (2017).
- **Frozen Virtual Natural Orbitals for Coupled-Cluster Linear-Response Theory**, **A. Kumar** and T.D. Crawford, J. Phys. Chem. A, 2017, 121 (3), 708-716.
- **Frozen-Density Embedding Potentials and Chiroptical Properties**, T.D. Crawford, **A. Kumar**, K.P. Hannon, S. Hoefener, and L. Visscher, J. Chem. Theory Comp. 11, 5305-5315 (2015).
- **Incremental evaluation of coupled cluster dipole polarizabilities**, J. Friedrich, H.R. McAlexander, **A. Kumar**, and T.D. Crawford, Phys. Chem. Chem. Phys. 17, 14284-14296 (2015).

Software Skills

Programming languages: **C/C++**, **Python**, **Bash**; Parallel Programming models: **OpenMP**, **MPI**
Version control: **Git**, **SVN**; Softwares: **Matlab**, **Mathematica**, **Latex** etc.