

# AJAY MELEKAMBURATH

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## EDUCATION

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**PhD in Chemistry**, Department of Chemistry, Virginia Tech 2022 - Present  
Computational chemistry and many-body electronic structure methods

**Integrated BS-MS**, Indian Institute of Science Education and Research Thiruvananthapuram 2016 - 2021  
Major in Chemistry with a minor in Physics

## RESEARCH EXPERIENCE

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**Graduate Student** Aug 2022 - Present  
Advisor: Prof. Edward F. Valeev, Virginia Tech

- Investigating effects of higher-order correlation and relativistic corrections on ground and excited state properties.
- Automated implementation of general-order coupled-cluster methods for ground and excited states
- Development of **SeQuant**: a framework for the symbolic algebra of tensors over scalar and operator fields
- Development of **MPQC4**: a parallel distributed-memory electronic structure package built on **TiledArray**

**Research Assistant** Jun 2021 - Jun 2022  
Advisor: Prof. R. S. Swathi, Indian Institute of Science Education and Research Thiruvananthapuram  
Funded through the Nano Mission project, Department of Science and Technology, India

- Development and parametrization of empirical potentials from electronic structure calculations
- Inclusion of many-body effects, anisotropic effects, and higher-order dispersion terms in empirical potential formulations

**Master's Student** Jul 2020 - Apr 2021  
Advisor: Prof. R. S. Swathi, Indian Institute of Science Education and Research Thiruvananthapuram

- Investigation of interlayer interactions in graphyne bilayers
- Investigation of the effect of anisotropic terms in empirical potential formulations
- Development and parametrization of empirical potentials for graphyne bilayers from electronic structure calculations

## PUBLICATIONS

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1. **SeQuant** Framework for Symbolic and Numerical Tensor Algebra. II. Many-Body Quantum Simulation Features  
Ajay Melekamburath, Azam Besharatnik, Nakul Teke, Conner Masteran, Bimal Gaudel, Robert G Adam, Edward F. Valeev\* (*Manuscript under preparation*)
2. **SeQuant** Framework for Symbolic and Numerical Tensor Algebra. I. Core Capabilities  
Bimal Gaudel, Robert G. Adam, Ajay Melekamburath, Conner Masteran, Nakul Teke, Azam Besharatnik, Andreas Köhn, Edward F. Valeev\* *J. Chem. Phys.*, **2026**, 164(14)
3. Adsorption of Aromatic Hydrocarbons on Graphene: From Energy Decomposition to Stable Adsorption Geometries  
Megha Rajeevan, Ajay Melekamburath, Rotti Srinivasamurthy Swathi\*  
*Chem. Asian J.*, **2026**, 21(3), e70603

4. “Best” iterative coupled-cluster triples model? More evidence for 3CC  
Nakul Teke, Ajay Melekamburath, Bimal Gaudel, Edward F. Valeev\*  
*J. Phys. Chem. A*, **2024**, 128 (45), 9819-9828
5. A Journey towards the heaven of chemical fidelity of intermolecular force fields  
Anto James<sup>†</sup>, Chris John<sup>†</sup>, Ajay Melekamburath, Megha Rajeevan and Rotti Srinivasamurthy Swathi\*  
*Wiley Interdiscip. Rev. Comput. Mol. Sci.*, **2022**, e1599
6. In pursuit of accurate interlayer potentials for twisted bilayer graphynes  
Ajay Melekamburath, Anto James, Megha Rajeevan, Chris John and Rotti Srinivasamurthy Swathi\*  
*Phys. Chem. Chem. Phys.*, **2021**, 23, 27031-27041

## CONFERENCES AND TALKS

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### Poster Presentations

1. Modern Wavefunction-Based Methods in Electronic Structure Theory Summer School 2025, University of Pisa, Italy
2. Annual Meeting of the Southeastern Theoretical Chemistry Association (SETCA) 2025, University of Memphis, Memphis, USA
3. American Conference on Theoretical Chemistry (ACTC) 2024, University of North Carolina, Chapel Hill, USA
4. Annual Meeting of the Southeastern Theoretical Chemistry Association (SETCA) 2024, Virginia Tech, Blacksburg, USA
5. Theoretical Chemistry Symposium (TCS) 2021, IISER Kolkata, India
6. DAE Symposium on Current Trends in Theoretical Chemistry (CTTC) 2020, Bhabha Atomic Research Centre, Mumbai, India
7. RSC-IISER Desktop Seminar with PCCP, Royal Society of Chemistry and Indian Institute of Science Education and Research Thiruvananthapuram, India

## TEACHING EXPERIENCE

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**Graduate Teaching Assistant**, Department of Chemistry, Virginia Tech Aug 2022 - April 2023

Course: General Chemistry Lab

Developed and delivered weekly presentations for undergraduate students. Supervised over 70 students doing experiments and preparing scientific reports. Evaluated the reports and gave feedback to students to help them develop writing skills.

## TECHNICAL SKILLS

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Programming languages      Modern C++ , Python, Bash, CUDA (basic)

Libraries                      Boost, Eigen

Other tools                     CMake, Git, GitHub Actions

## ACHIEVEMENTS & AWARDS

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**Innovation in Science Pursuit for Inspired Research (INSPIRE) Fellowship** 2016 - 2021

Department of Science and Technology, India

Amount: ~ \$6000