AJAY MELEKAMBURATH

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EDUCATION

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

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

- 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`
- Automated implementation of higher-order coupled-cluster methods for ground and excited states

Research Fellow Jun 2021 - Jun 2022
Advisor: Dr. 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: Dr. 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

1. From energy decomposition to stable adsorption geometries: a study of polycyclic aromatic hydrocarbon-graphene interactions
   Megha Rajeevan, Ajay Melekamburath, Rotti Srinivasamurthy Swathi* (*Manuscript under preparation*)
2. "Best" iterative coupled-cluster triples model? More evidence for 3CC
   Nakul Teke, Ajay Melekamburath, Bimal Gaudel, Edward F. Valeev*
   J Phys. Chem. A, **2024**, 10.1021/acs.jpca.4c04667
3. A Journey towards the heaven of chemical fidelity of intermolecular force fields
   Anto James†, Chris John†, Ajay Melekamburath, Megha Rajeevan and Rotti Srinivasamurthy Swathi*
   Wiley Interdiscip. Rev. Comput. Mol. Sci., **2022**, e1599
4. 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

Poster Presentations

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

TEACHING EXPERIENCE

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

Programming languages	C++, Python, Bash
Other tools	Psi4, Gaussian, Git

ACHIEVEMENTS & AWARDS

Innovation in Science Pursuit for Inspired Research (INSPIRE) Fellowship 2016 - 2021
Department of Science and Technology, India
Amount: $\sim$ \$6000