AJAY MELEKAMBURATH

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EDUCATION

PhD in Chemistry, Department of Chemistry, Virginia Tech 2022 - Present

Integrated BS-MS, Indian Institute of Science Education and Research Thiruvananthapuram 2016 - 2021
Major in Chemistry with minor in Physics
GPA: 7.56/10

RESEARCH EXPERIENCE

Graduate Student Aug 2022 - Present
Advisor: Prof. Eduard Valeyev, Virginia Tech

- Working on efficient implementation of electronic structure methods

Research Fellow Jun 2021 - Jun 2022
Indian Institute of Science Education and Research Thiruvananthapuram
Funded through 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 Thesis 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 potential for graphyne bilayers from electronic structure calculations

PUBLICATIONS

1. 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**
2. 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

PRESENTATIONS

Poster Presentations

1. Ajay Melekamburath, Anto James and R. S. Swathi, In pursuit of of accurate model potentials for twisted bilayer graphynes
   17^{th} Theoretical Chemistry Symposium (TCS-2021), IISER Kolkata, India
2. Ajay Melekamburath, Anto James and R. S. Swathi, In pursuit of of accurate model potentials for twisted bilayer graphynes
   DAE Symposium on Current Trends in Theoretical Chemistry (CTTC-2020), Bhabha Atomic Research Centre, Mumbai, India

3. Ajay Melekamburath, Anto James and R. S. Swathi, In pursuit of of accurate model potentials for twisted bilayer graphynes
   RSC-IISER Desktop Seminar with PCCP, Royal Society of Chemistry and IISER TVM, India

TEACHING EXPERIENCE

Graduate Teaching Assistant, Department of Chemistry, Virginia Tech Aug 2022 - Present
Course: General Chemistry Lab
Developed and delivered weekly presentations for three sections of 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, HTML, CSS
HPC	SLURM Workload Manager, PBS
Other tools	Gaussian, Psi4, Mathematica, Git

ACHIEVEMENTS & AWARDS

Innovation in Science Pursuit for Inspired Research (INSPIRE) Fellowship 2016 - 2021
Department of Science and Technology, India
Amount: $\sim$ $4000