

Ajay Melekamburath

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Education

Indian Institute of Science Education and Research Thiruvananthapuram

Kerala, India

Integrated BS-MS, Major in Chemistry with Minor in Physics

August 2016 - July 2021

- CGPA of 7.65/10

Ideal Higher Secondary School Dharmagiri (Grade 12)

Kerala, India

Higher Secondary - Kerala Board of Public Examinations

June 2014 - April 2016

- 97.8% marks in Chemistry, Physics, Mathematics and Biology

Govt. Higher Secondary School Peruvallur (Grade 10)

Kerala, India

Secondary - Kerala Board of Public Examinations

April 2014

- 95% marks in Chemistry, Physics, Mathematics, Biology and Social Sciences

Research Experience

Improving the fidelity of intermolecular potentials: from molecular aggregates to van der Waals heterostructures

Guide: Dr. R. S. Swathi

Short Term Project: June 2021 - Present

School of Chemistry, IISER TVM

Reviewed the advances made in the development of empirical potentials, such as inclusions of many-body effects, anisotropic effects and higher-order dispersion terms in potential formulations, to address non-covalent interactions in structures ranging from molecular clusters to van der Waals heterostructures. (Article published in *Wiley Interdiscip. Rev. Comput. Mol. Sci.* - DOI: 10.1002/wcms.1599)

Modeling of twisted bilayer graphynes using empirical potentials

Guide: Dr. R. S. Swathi

Master Thesis Project: July 2020 - April 2021

School of Chemistry, IISER TVM

Investigated the effects of twisting on interlayer separation and cohesion energy of graphyne bilayers. Empirical potentials were parametrized for graphyne bilayers, taking high level dispersion-corrected density functional theory calculations as benchmarks. Isotropic and anisotropic potentials were compared and the importance of anisotropic effects while modeling tribological properties was highlighted. (An article based on this work has been published in *Phys. Chem. Chem. Phys.* - DOI: 10.1039/D1CP03637H)

Quantum computation of electronic transitions using Multistate Contracted Variational Quantum Eigensolver

Guide: Prof. Anil Shaji

Minor Research Project: December 2019 - July 2020

School of Physics, IISER TVM

An implementation of the multistate contracted variational quantum eigensolver algorithm (MC-VQE) for calculating electronic transitions was studied. An ab initio exciton model was used to model a 18-monomer chromophore system.

Electronic structure modeling of twisted bilayer graphynes

Guide: Dr. R. S. Swathi

Summer Research Project: May 2019 - July 2019

School of Chemistry, IISER TVM

Studied the variation of interaction energy with the interlayer separation and twist angle of bilayer graphynes. Familiarized with Gaussian 16 and GaussView, and carried out density functional theory calculations.

Introduction to electronic structure theory

Guide: Dr. R. S. Swathi

Reading Project: December 2018

School of Chemistry, IISER TVM

Reading project on modern electronic structure theory. Learned about the basics of wavefunction methods. Reference: Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Attila Szabo, Neil S. Ostlund

A study on effect of degree of fermentation on insect attraction

Guide: Dr. Ullasa Kodandaramaiah

Laboratory Research Project: August 2016 - November 2016

School of Biology, IISER TVM

Carried out a series of experiments with various food samples for attracting insects in different habitats. Set up multiple insect traps around the IISER TVM campus.

Publications

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** (DOI: 10.1002/wcms.1599)

([‡] A. J. and C. J. contributed equally.)

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

Research Interests

- Theoretical Method Development and High-throughput Computational Methods: Development of theoretical models which can take advantage of the rapid advancements in computational power, and their implementation into efficient computer programs.
- Application of these novel methods to address problems in the broad area of chemistry, especially regarding the non-covalent interactions between molecular species.

Achievements

Standard Test Scores

2020 **TOEFL - Internet Based Test: 105/120**

Reading: 29/30, Listening: 29/30, Speaking: 23/30, Writing: 24/30

Scholarships

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

Department of Science and Technology, India.

2014 **National Means Cum-Merit Scholarship (NMMS)**

Govt. of India.

2011-2014 **Promotion of Excellence among Gifted Children (PEGS)**

Govt. of Kerala.

Awards

2018 **State Level Topper - Mimamsa 2018 - National-level Intercollegiate Quiz**

Indian Institute of Science Education and Research Pune

2016 **All India Rank: 196 - All India Entrance Examination for Admission (AIEEA-UG)**

Indian Council of Agricultural Research

2016 **All India Rank: 610 - Common Admission Test (CAT) 2016**

Cochin University of Science and Technology (CUSAT)

2016 **State Level Rank: 1080 - Kerala Engineering Architecture Medical (KEAM) Entrance Exam**

Govt. of Kerala.

Skills

Computational & Software Skills

- **Programming Languages:** Python, Bash, Mathematica, MATLAB, HTML5, CSS
- **Softwares and Programs:** Gaussian 16, Quantum Espresso, GaussView, xCrySDen, SLURM Workload Manager, TORQUE, LaTeX, IBM's Qiskit, OriginPro, Blender, Adobe Photoshop, Adobe InDesign

Languages

- **Malayalam** - Native proficiency, **English** - Professional proficiency & **Hindi** - Conversational proficiency

Conferences & Workshops

- Aug 2021 **International Workshop on High-Performance Computing in Science and Engineering**
Centre of High-Performance Computing, IISER TVM
- Feb 2020 **IISER TVM - RSC Symposium on Advances in Chemical Sciences**
Royal Society of Chemistry and IISER TVM
- Feb 2020 **Quantum Computing Workshop**
Dhwani 2020, College of Engineering Thiruvananthapuram
- Jan 2020 **Frontier Symposium in Chemistry 2020 (FS-CHM 2020)**
School of Chemistry, IISER TVM
- Jun 2019 **Workshop in Theoretical Chemistry**
NPTEL India, IISER Pune

Poster Presentations

- Dec 2021 **Title: In pursuit of accurate model potentials for twisted bilayer graphynes**
17th Theoretical Chemistry Symposium (TCS-2021), IISER Kolkata, India.
- Sept 2021 **Title: In pursuit of accurate model potentials for twisted bilayer graphynes**
DAE Symposium on Current Trends in Theoretical Chemistry (CTTC-2020), Bhabha Atomic Research Centre, Mumbai, India.
- May 2021 **Title: In pursuit of accurate model potentials for twisted bilayer graphynes**
RSC-IISER Desktop Seminar with PCCP, Royal Society of Chemistry and IISER TVM

Extracurricular Activities

Positions of Responsibility

- 2020-2021 **Secretary of Cultural Council**, Student Affairs Council, IISER TVM
- 2019 **Leading Member**, Production and Media Team - Inter IISER Cultural Meet (IICM) 2019
- 2018-2021 **Founding Member**, Media Society, IISER TVM
- 2018-2020 **Core Member**, Unnat Bharat Abhiyan Cell, IISER TVM, Govt. of India
- 2018-2020 **Organiser and Volunteer**, Ek Bharat Shreshth Bharat (EBSB) Initiative, Govt. of India
- 2017-2020 **Core Member**, Ishya '17, '18, '19 and '20 - the cultural fest of IISER TVM
- 2016-2019 **Member**, Cultural Council, IISER TVM
- 2016-2018 **Committee Member**, Student Co-operative Mess, IISER TVM

Avocations

- Amateur photographer: Travel, portrait and event photography
- Avid follower of football, FC Barcelona fan