Addanki Raghavendra

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Education

- **National Institute of Technology Calicut** Calicut, India
  Bachelor of Technology in Chemical Engineering; GPA: 9.09/10 *July 2019 – Present*
- **IIT Ramaiah Study Circle** Hyderabad, India
  Telangana State Board of Intermediate Education (TSBIE); Percentage: 96.4% *2017 – 2019*
- **Atomic Central School II Hyderabad** Hyderabad, India
  Central Board of Secondary Education; GPA: 10/10 *2016 – 2017*

Experience

- **International Centre for Clean Water** Chennai, India
  Research Intern, Supervisor: Dr. Ganapati Natarajan *December 2021 – Present*
  Research: DFT study on nanomaterial sensors for applications in water purification
  - Investigated the site-selectivity and bonding of analyte ions in water to electrochemically reduced graphene-oxide ERGO membrane using DFT calculations.
  - Constructed and performed geometry optimization for rectangular, flake, and stack rGO membrane structures.
  - Computed molecular visualizations of the steps for discovered ERGO-analyte ion mechanism.
  - Software tools: GPAW, ASE, DFTB+, VMD
  - Packages: ASE, Matplotlib
- **International Centre for Clean Water** Chennai, India
  Remote Research Intern, Supervisor: Dr. Ganapati Natarajan *August 2021 – Present 2021*
  Research: Molecular simulations in topology of gold-thiolate clusters
  - Working on investigating the topology of hybrid nanoclusters by developing optimization algorithms to predict stable configuration.
  - Performed structural analysis of few monolayer protected gold nanoclusters by decomposing the structure into mathematical cycles to predict the stable topology.
  - Conducted a literature survey on mechanically interlocked molecular architectures (MIMAs - catenane, rotaxane, borromean rings, knot, and clippane) and their applications.
  - Software tools: DFTB+, VMD, Avogadro
  - Packages: ASE, Matplotlib, Scipy, PyKnot, Networkx
- **Indian Institute of Technology Madras** Chennai, India
  Remote Research Intern, Supervisors: Prof. T. Pradeep *March 2021 – May 2021*
  Project: Hydroinformatics platform to analyze the problem of arsenic contamination in the state of Punjab
  - Conducted a literature survey on the water purification applications of a nanomaterial designed at Dr. T. Pradeep's Research Group to eliminate arsenic contaminants from water efficiently and cost effectively (0.35$/1000L water).
  - Worked with ArcGIS Pro and data visualizations tools such as Tableau & PowerBI to analyze the water quality data of all 22 districts in Punjab.
  - Performed correlation analysis among the parameters and investigated the notable correlations discovered.
- **National Institute of Technology Calicut** Calicut, India
  Undergraduate Researcher, Supervisor: Dr. N. Sandhyarani *Feb 2021 – Present*
  Research Work: Synthesis of nanomaterials and nanocomposites for their applications in clean energy
  - Currently hold a undergrad research position at Nanoscience Research Laboratory (NSRL), NIT Calicut.
  - Working with advanced imaging techniques used for studying the structure-property relationship of synthesized nanomaterials and modified surfaces.
  - Worked on characterizing various nanomaterials using spectroscopy, microscopy and electrochemcial techniques. And experimented the uses of these nanomaterials in methanol biofuels.

Independent Projects

- **Numerical analysis of molecular dynamics for L-J particles in 3D**
  Software used: LAMMPS, MATLAB

Relevant Coursework

- Physical Chemistry, Material Science, , Quantum Physics, Thermodynamics, Computational Methods In Engineering, Fluid Mechanics, Machine Learning for Data Science & Analytics, *Materials Modelling Course 2021_22(Thomas Young Centre TYC), *Atoms to Materials: Predictive Theory and Simulations(edX), *Advanced Thermodynamics and Molecular Simulations (NPTEL) [*refers to online coursework]

Academic Highlights

- **GPA:** GPA - 9.09/10, IIIrd Semester GPA - **9.7/10**; Secured top GPA thrice in my five semesters of study
- **Joint Entrance Examination:** Secured 98.41 percentile in the JEE (Mains) Examination of 2019
- **Telangana State Engineering, Agriculture and Medical Common Entrance Test (TS-EAMCET):** Secured top 0.2% rank in the TS-EAMCET Examination of 2019
- **National Talent Search Examination (NTSE) Stage-I:** Cleared the National Talent Search Examination (top 99.38%) conducted in 2017

Publications

- Sourav Jana, Md. Rabiul Islam, Ganapati Natarajan, **Addanki Raghavendra**, Chennu Sudhakar, Thalappil Pradeep. "A selective arsenite sensor in the field at 10 ppb with a mobile phone", *Journal of Chemical Theory and Computation* (Under Review)

Competitions

- **Hindustan Petroleum NGIC (New Generation Ideation Contest) 2021:** Finalist in the All India Under Graduate Category for NGIC-2021 conducted by HP Green R&D Centre Bangalore (results yet to be announced)

PSM Certifications

- "***Laboratory Safety***" – a safety and chemical engineering education program by AICHE Academy. Credential.
- "***An Introduction to Managing Process Safety Hazards***" – a safety and chemical engineering education program by AICHE Academy. Credential.

Mentorships

- **Student Mentor:** Academic Mentor at Ignite Club, NIT Calicut. Mentored seven students from Kerala government secondary schools to help them prepare for the Joint Entrance Examination (JEE).
- **Sports Mentor:** Kho-kho mentor for the Institute Juniors Kho-kho team.

Attended Workshops/Webinars

- Machine Learning at the Atomic Scale - Chemical Reviews Thematic Talk Series (ACS): 22 September 2021
- MolSimEng Workshop 2021: 24 September 2021
- Cecam Mixed-gen Season 2: Started on 27 October 2021
- iRASPA/RASPA Online Workshop 2022: 20 January 2022
- Cecam Virtual Winter School on Computational Chemistry: 21 - 25 February 2022

Other Experience

- **Tathva - NIT Calicut:** Member of Tathva Content Creation Committee; Marketing Executive at Tathva. Tathva is South India's largest Techno-Management Fest.
- **Compter Skills:** Unix Shell, Python, MATLAB, Machine Learning, LaTeX
- **Materials modeling tools:** DFTB+, Lammps, VMD, Avogadro, Aiida Workflow
- **Special Research Interests:** First-Principles Modeling, Materials Informatics, Physics-inspired ML
- **Personal Interests:** Playing kho-kho, Cooking, Traveling