Sundaresan Ravi

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PERSONAL STATEMENT

As an undergraduate in Chemistry with a strong interest in theoretical and computational chemistry, I am driven by the interdisciplinary of computational chemistry techniques. My experience with **Density functional theory (DFT) calculations using VASP** and **Gaussian** has equipped me with a robust skill sets for tackling diverse computational projects. I am particularly fascinated by the **potential of machine learning to advance our understanding of spectroscopic properties**. I am eager to apply my skills in an internship program that involves developing **innovative computational strategies** and **machine learning models** to support various research fields. Joining your esteemed group would allow me to contribute to cutting-edge projects in computational chemistry, collaborate with leading experts, and make meaningful advancements in this field.

EDUCATION

SRM University, College of Science and Humanities | Chennai, India 2022-2026

Bachelors of Science

General Chemistry

GPA: 8.79/10 (as of 5th Semester)

RESEARCH INTERESTS

- Scientific programming
- Density Functional Theory (DFT)
- Quantum Chemical Calculations and Modeling
- Machine learning

RESEARCH PROJECTS

1. Enhancing Supercapacitive Performance of WS_2 via Transition Metal Intercalation (Completed)

Supervisor: Dr. Tumpa Sadhukhan, Research Assistant Professor, Department of Chemistry, SRM-IST

- **Objective:** Investigated the effect of transition metal intercalation on WS_2-based supercapacitors.
- **Contributions:**
  - Conducted DFT calculations using VASP.
  - Developed code for calculating the quantum capacitance using Python.

2. Application of Machine learning to predicting spectroscopic properties of transition metal complexes (ongoing)

Supervisor: Dr. Tumpa Sadhukhan, Research Assistant Professor, Department of Chemistry, SRM-IST

- **Objective**: Prediction of spectroscopic properties of transition metal complexes for photodynamic therapy
- **Contributions**:
    - Creating dative bonded smiles of transition metal complexes
    - I have created and curated a database of transition metal complexes by employing Gaussian codes for geometry optimization and property calculations, tailored for use in predictive modeling applications

WORKSHOPS, CONFERENCES AND COURSES ATTENDED

- **Material Informatics: Fingerprints, Graph Neural Networks and Transformer-Based Models for Materials Design,** Venue: Indian Institute of Technology Madras (20th-24th January 2025) - *Participant*
- **Computational Chemistry techniques –** NPTEL+**,** Venue: Online (18th-19th January 2025) - *Participant*
- **Hands-On Workshop on Density Functional Theory (DFT) Calculations,** Venue: Online (1st -7th September 2024) - *Participant*
- **Hands-On Workshop on Molecular Docking & MD Simulation: From Theory and Practical,** Venue: Online (1st -7th September 2024) - *Participant*
- **Modern computational chemistry and AI with MLatom@XACS – XACS Cloud,** Venue, Online
- **AI and Machine Learning in Material Science,** Venue: Indian Institute of Technology Madras (7th-9th June 2024) - *Participant*
- **Computational Methods for Solving Chemical problems**, Venue: National Institute of Technology Trichy (21st-22nd February 2024) - *Participant*
- **ASTON'S Workshop on Mass Spectrometry,** Venue: SRM Institute of Science and Technology (25th - 26th August 2023) - *Participant*

TECHNICAL AND LANGUAGE SKILLS

Technical and Soft:

- Basic Proficiency in **Vienna Ab initio Simulation Package (VASP) and Gaussian to perform DFT calculations**.
- Basic proficiency in Scientific Programming (**Python, RDKit**).
- Strong communication and interpersonal skills.
- Effective time management and adaptability.
- Good at Team-oriented and independent contributions.

Language:

- Fluent in English and Tamil.

REFERENCE

- Dr. Tumpa Sadhukhan, Department of Chemistry, College of Engineering & Technology, SRM Institute of Science and Technology, Kattankulathur, Chennai-603203, India. Email: tumpas@srmist.edu.in (Relationship: Project-Advisor)