Sai Vijay Bhaskar Mocherla

Graduate Student (2023 - Present)
Surface Dynamics Group
Tata Institute of Fundamental Research (TIFR)
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EDUCATION

M.S. in Chemistry **August 2020**
University of Rochester, USA
CGPA: 3.72/4.00

M.Sc. in Chemistry **April 2019**
Sri Sathya Sai Institute of Higher Learning (SSSIHL), Prasanthi Nilayam, India
CGPA: 8.2/10.0
Thesis: Effect of Torsional Disorder on Exciton Migration in Conjugated Polymers

B.Sc. (Honors) in Chemistry **April 2016**
Sri Sathya Sai Institute of Higher Learning (SSSIHL), Bangalore, India
CGPA: 7.3/10.0 (Major's CGPA: 7.65/10.0)

RESEARCH EXPERIENCE

Graduate Student, Tata Institute of Fundamental Research, Hyderabad **02/2024 - Present**

Advisor: Prof. Pranav R. Shirhatti, TIFR Hyderabad
- Research Focus: Understanding chemical reaction dynamics in surface chemistry through molecule-surface scattering experiments.
- Lab rotation project: Calculated the vibrational excitation probability for preparation of state specific gas-phase reagents using single mode continuous wave (cw) lasers. Additionally, a parallelised C++ program (rap-mb) to perform Monte Carlos simulations of rapid adiabatic passage in molecular beams was also developed.

Junior Research Fellow, Tata Institute of Fundamental Research, Hyderabad **09/2021 - 05/2023**

Advisor: Prof. Raghunathan Ramakrishnan, TIFR Hyderabad
- Studied the effects of electron correlations on ultrafast electron dynamics in atoms and molecules using time-dependent ab initio methods.
- Developed a method to prepare hybrid Gaussian basis sets optimized for calculating higher harmonic (HHG) spectra using the time-dependent configuration interaction (TDCI) approach.

Summer Project Student, University of Rochester, New York, USA **05/2020 - 11/2020**

Advisor: Prof. Andrew Jordan, Department of Physics and Astronomy
- Studied low-temperature physics of vortex-matter phases in type-II superconductors to develop quantum refrigeration schemes that use fluxons as heat carriers.

Visiting Student, Tata Institute of Fundamental Research, Mumbai **04/2018 - 06/2018**

Advisor: Prof. Venu Gopal Achanta, Department of Condensed Matter Physics and Material Science
- Worked on design of optical nanostructures with dispersion-less plasmon modes, and their fabrication on gold thin films using e-beam lithography and other cleanroom techniques.
- Studied the emergence of broadband optical transmission in 'plasmonic quasi-crystals' using angle-resolved optical transmission measurements. Assisted in setting up the multi-color pump-probe spectroscopy apparatus to measure the lifetimes of charge carriers(hot electrons) in fabricated optical nanostructures.

TEACHING EXPERIENCE

Teaching Assistant, Department of Chemistry, University of Rochester **08/2019 - 04/2020**

- Organized demonstrations of experiments and supervised lab sessions for freshman General Chemistry (CHEM-131L) during fall '19 semester.
- Conducted problem solving sessions and discussion workshops as a graduate TA (workshop leader) for Physical Chemistry: Thermodynamics, Statistical Mechanics, and Kinetics (CHEM-252) during spring '20 semester.

TECHNICAL SKILLS

Programming and Software: Python, Fortran, C++ and Mathematica

- Proficient in numpy, scipy, matplotlib, pandas, cython, scikit-learn and pybind11.
- Linux shell scripting, BLAS, LAPACK, CMake
- Ab initio packages: Gaussian, NWChem, Psi4 and PySCF.

Experiments:

- Trained in design and fabrication of optical nanostructures using e-beam lithography.
- Skilled in wet chemistry and clean room techniques, including thin-film deposition, sputtering, etching.

PUBLICATIONS/PRE-PRINTS

- Mocherla, Sai Vijay, and Raghunathan Ramakrishnan. "Variational augmentation of Gaussian continuum basis sets for calculating atomic higher harmonic generation spectra." arXiv preprint arXiv:2307.00732 (2023).

RELEVANT COURSEWORK

- **Undergraduate Courses**:
  Calculus, Vector Analysis, Probability, Ordinary and Partial Differential Equations, Linear Algebra.
  Classical mechanics, Electromagnetism, Optics, Electronics.
  Quantum Chemistry, Physical Chemistry, Analytical Chemistry, Chemical Kinetics.
- **Graduate Level Courses:**
  (University of Rochester)
  Quantum Mechanics, Mathematical Methods, Quantum Optics,
  Quantum Dynamics, Statistical Mechanics, Modern Statistics and Data Exploration in Physics
  (TIFR Hyderabad)
  Molecular Dynamics, Spectroscopy of atoms and molecules, Condensed Matter Physics.
