SAI VIJAY BHASKAR MOCHERLA

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EDUCATION

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

M.Sc. in Chemistry   **April 2019**
 Sri Sathya Sai Institute of Higher Learning (SSSIHL), Prasanthi Nilayam, India
 CGPA: 8.2/10.00
 Thesis: Effect of Torsional Disorder on Exciton Migration in Conjugated Polymers

B.Sc. (Hons.) 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)

SKILLS

Programming and Software: Python, Fortran, C/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.
 - Developed a scientific computing package in python and C++ to run laser-driven electron dynamics simulations on HPC systems.

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.

RESEARCH EXPERIENCE

Junior Research Fellowship, Tata Institute of Fundamental Research, Hyderabad   09/2021 - 05/2023
Advisor: Prof. Raghunathan Ramakrishnan, TIFR Center for Interdisciplinary Sciences (TCIS)
 - 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.
 - Pre-print: "Variational augmentation of Gaussian continuum basis sets for calculating atomic higher harmonic generation spectra" arXiv:2307.00732 (2023).

Summer Research Project, 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.

Research Internship, Indian Institute of Science, Bangalore   05/2019 - 07/2019
Advisor: Prof. Upendra Harbola, Department of Inorganic and Physical Chemistry (IPC)
 - Modeled transport of quasiparticles in nano materials using different Random-walk mechanisms

M.Sc. Research Project, Sri Sathya Sai Institute of Higher Learning, India 08/2018 - 02/2019

<u>Advisor</u>: Dr. B Siva Kumar, Department of Chemistry

- Developed a theoretical model of an exciton coupled to torsional modes of a polymer subunit to study the effects of torsional disorder on exciton transport in conjugated polymers.
- Built numerical routines to evaluate the disorder-averaged intramolecular exciton migration rates to study their scaling properties with the increasing length of the polymer chain.

Summer Internship (VSRP), Tata Institute of Fundamental Research, Mumbai 04/2018 - 06/2018

<u>Advisor</u>: 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.

Research Internship, Sri Sathya Sai Institute of Higher Learning, India 11/2017 - 02/2018

<u>Advisor</u>: Prof. Sai Sathish Ramamurthy, Department of Chemistry

- Worked on fabrication of polymer thin-film nano-gratings using Fracture induced-structuring (FIS) for surface-plasmon enhanced fluorescence sensing applications.

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.

SOME RELEVANT COURSEWORK

- <u>**Undergraduate Courses**</u>:
  Calculus, Vector Analysis, Probability, Ordinary and Partial Differential Equations, Linear Algebra.
  Classical mechanics, Electromagnetism, Optics, Electronics.
- <u>**Graduate Level Courses:**</u> (at University of Rochester)
  Quantum Mechanics, Mathematical Methods, Quantum Dynamics, Statistical Mechanics,
  Modern Statistics and Data Exploration in Physics.