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, pandas, cython, scikit-learn, matplotlib.
 - Linux shell scripting, BLAS, LAPACK, CMake
 - Ab initio packages: Gaussian, NWChem, Psi4 and PySCF.
 - Developed a scientific computing package in python and C++ to efficiently perform time-dependent configuration interaction (TDCI) simulations for laser-driven electron dynamics.

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 Fellow, Tata Institute of Fundamental Research, Hyderabad **09/2021 - 05/2023**
Advisor: Prof. Raghunathan Ramakrishnan, TIFR Center for Interdisciplinary Sciences (TCIS)
 - Developed a scientific computing package written in python and C++, for performing time-dependent configuration interaction (TDCI) calculations. Optimized hybrid Gaussian basis sets for calculating higher harmonic (HHG) spectra using the 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 time-dependent Ginzburg-Landau models to understand vortex transport and low-temperature physics of vortex-matter phases in type-II superconductors for quantum refrigeration applications.

Research Intern, 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>: Prof. 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.
- Numerically evaluated disorder-averaged intramolecular exciton migration rates were found to scale inversely with the increasing length of the polymer chain.
- Built numerical routines to simulate the quantum dynamics and explored the implementation of Tensor Network methods (based on DMRG) to handle quantum entanglement with increasing system size.

Summer Research Fellow, 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 Intern, 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.
- **<u>Graduate Level Courses</u>:** (at University of Rochester)
  Quantum Mechanics, Mathematical Methods, Quantum Dynamics, Statistical Mechanics, Modern Statistics and Data Exploration in Physics.