SAI VIJAY BHASKAR MOCHERLA

Junior Research Fellow, MOLDIS-Group

TIFR Center for Interdisciplinary Sciences(TCIS)

Tata Institute of Fundamental Research

Email: vijaysai.mocherla@gmail.com
Website: vijaymocherla.github.io

Hyderabad, India

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)

RESEARCH EXPERIENCE

Junior Research Fellow, Tata Institute of Fundamental Research, Hyderabad 09/2021 - present

Advisor: Prof.Raghunathan Ramakrishnan, TIFR Center for Interdisciplinary Sciences(TCIS)

- Using configuration interaction methods to study electron-correlation effects in molecules that can be challenging to capture with TD-DFT using approximate functionals.

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

- 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

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 these 'plasmonic quasi-crystals' using angle-resolved optical transmission measurements.
- Assisted in setting up the multi-color pump-probe spectroscopy apparatus to further 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

Advisor: 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.

SKILLS

Programming and Software: Python and Mathematica

- Python: Numpy, SciPy, Pandas, Cython, Scikit-learn, Matplotlib, SymPy.
- Basic (used for a project/course): Fortran, C/C++, Octave, Javascript, CSS, HTML
- Computational(ab initio packages): Gaussian, NWChem, PSI4.

Nano Fab:

- 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.

TEACHING EXPERIENCE

Teaching Assistant, Department of Chemistry, University of Rochester

08/2019 - 04/2020

- Organized and supervised lab sessions for freshman General Chemistry(CHEM-131L) in fall '19
- Led problem solving and workshop for undergraduate and graduate students taking the course: Physical Chemistry-II: Thermodynamics and Statistical Mechanics (CHEM-252).

ACADEMIC ACHIEVEMENTS

- Qualified the 'IIT JEE Mains' in 2013 within the top 90 percentile (a National-level entrance test for undergraduate admissions in Science and Engineering).
- Qualified the IIT JAM, Chemistry in 2017 and GATE Chemistry in 2019 within 95 percentile. (National-level entrance tests for masters and Ph.D. admissions).

SOME RELEVANT COURSEWORK

- MATHEMATICS: Multivariable Calculus, Vector Analysis, Theory of Probability, Theory of Ordinary and Partial Differential Equations, Linear Algebra and Boundary Value Problem
- PHYSICS:

<u>Graduate Level Courses</u>: (at University of Rochester) Quantum Mechanics, Mathematical Methods for Physics and Optics, Quantum Optics, Quantum Dynamics, Statistical Mechanics, Modern Statistics and Data Exploration in Physics.

<u>Undergraduate Courses</u>: Classical Mechanics, Electricity and Magnetism, Electronics, Optics.

- CHEMISTRY:

Masters Courses: Advanced aspects of Physical Chemistry, Quantum Chemistry, Thermodynamics and Statistical Mechanics, Computational Chemistry, Molecular Spectroscopy, Advanced aspects of Group Theory, Polymers Chemistry, Bio-Catalysis, Organic Structure and Stereochemistry

<u>Undergraduate Courses:</u> Fundamentals of Theoretical chemistry, Physical Chemistry, Inorganic Chemistry, Organic Chemistry and Biochemistry