

## SAI VIJAY BHASKAR MOCHERLA

Junior Research Fellow, [MOLDIS-Group](#)  
TIFR Center for Interdisciplinary Sciences (TCIS)  
Tata Institute of Fundamental Research  
Hyderabad, India

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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)

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### RESEARCH EXPERIENCE

#### Junior Research Fellow, Tata Institute of Fundamental Research, Hyderabad

09/2021 - present

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

- Currently investigating ultra-fast electron dynamics in atoms and molecules using time-dependent ab initio methods from quantum chemistry.

#### 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

Advisor: 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

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.

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.
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## **SKILLS**

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

- Python: Numpy, SciPy, Pandas, Cython, Scikit-learn, Matplotlib, SymPy.
- Basic: Linux shell scripting, BLAS, LAPACK, Javascript, CSS, HTML
- Ab initio packages: Gaussian, NWChem, PSI4 and PySCF.

**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.
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## **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.
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## **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:**
    - Graduate Level Courses: (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.
    - Undergraduate Courses: 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
    - Undergraduate Courses: Fundamentals of Theoretical chemistry, Physical Chemistry, Inorganic Chemistry, Organic Chemistry and Biochemistry
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