## SAI VIJAY BHASKAR MOCHERLA

Junior Research Fellow, Moldis-Group

TIFR Center for Interdisciplinary Sciences(TCIS)

Tata Institute of Fundamental Research

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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

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 07/2021 - 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

**April 2016** 

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
- Illustration and Graphics: Blender and Adobe Creative Cloud.
- 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:

<u>Masters Courses:</u> 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