

## Rithwik Tom

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## Education

**Carnegie Mellon University (CMU), Pittsburgh, USA - 15213** August 2017 - Present

Course : Ph.D. (Physics)  
CGPA : 3.86/4.33  
Faculty Advisor : Asst. Prof. Noa Marom

**Indian Institute of Science (IISc), Bangalore, India - 560012** August 2013 - May 2017

Course : Bachelor of Science (Physics)  
CGPA : 6.6/8  
Faculty Advisors : Prof. Rahul Pandit and Dr. Samriddhi Shankar Ray  
Thesis : Statistical Properties of Shell Models in Fluid Turbulence

## Research Interests

- Molecular Crystal Structure Prediction
- Ab-initio Electronic Structure Methods
- High Performance Computing (HPC)

## Research Experience

**Genarris 2.0: Random Crystal Structure Generator** CMU, August 2018 - Present

Developed Genarris 2.0, a random molecular crystal structure generator for seeding crystal structure prediction algorithms and training machine learning models. Implemented fast algorithms to ensure physical constraints, detect symmetries of molecules and to align them on special positions of space groups. Parallelized using MPI and OpenMP. *Written in:* C, Python.

**Singlet Fission in Phenylated Acenes** CMU, May 2018 - December 2018

Electronic and excitonic properties of tetracene, pentacene, and their phenylated derivatives in the gas phase and solid state were investigated using many-body perturbation theory in the GW approximation and Bethe-Salpeter equation (BSE). Their potential for singlet fission was evaluated with respect to energy conservation criterion and the exciton charge transfer character.

**Statistical Properties of Shell Models in Fluid Turbulence** IISc, May 2014 - August 2014

Simulated shell models to study into the energy cascade phenomenon in fluid turbulence. Developed a code for a simplified shell model of turbulence to simulate and calculate two-point correlation functions of turbulent velocity fields. *Written in:* C++.

**Solving the Time-Dependent Schrödinger's Equation** NTU, May 2015 - July 2015

Developed a program to numerically solve the time-dependent Schrödinger's equation for simple time-varying potentials using split-step Fourier method and finite difference methods. Extended some schemes to include magnetic vector potentials. *Written in:* MATLAB.

## Awards

**KVPY Fellowship** August 2013 - May 2017

KVPY (Kishore Vaigyanik Protsahan Yogna) fellowship, funded by the Department of Science and Technology, India, is awarded to highly motivated undergraduates in basic sciences.

## Skills

- Programming and scripting languages: C, C++, MATLAB, Python, Bash.
- Parallel programming paradigms: Shared memory (OpenMP), distributed memory (MPI).
- Debuggers and profilers : GDB, Valgrind, Gprof.
- Version control system: Git.
- Ab-initio electronic structure codes: Quantum Espresso, FHI-aims, BerkeleyGW.

## Workshops

### **XSEDE HPC Workshop on MPI**

Pittsburgh, September 2019

Two day hands-on workshop on writing scalable codes using Message Passing Interface (MPI) in C and FORTRAN. Lectures on basic and advanced routines of the MPI standard.

### **Summer School and Workshop on Time Dependent DFT**

New Brunswick, August 2019

Methods and new developments in time-dependent density functional theory (TDDFT), which is employed for calculating excited state properties of molecule and solids. Hands-on session on TDDFT codes.

### **Recent Developments in Electronic Structure Theory**

Urbana-Champaign, May 2019

Lectures on recent developments and applications of electronic structure theory using density functional theory, molecular dynamics, Monte Carlo methods, and exascale computing.

### **Sixth Annual Workshop on BerkeleyGW**

Berkeley, June 2019

Lectures on theory, applications, and computational details of GW and Bethe-Salpeter calculations using BerkeleyGW. Hands-on tutorials for quasiparticle and optical properties of solids, molecules and nanosystems.

### **Fifth Annual Workshop on BerkeleyGW**

Berkeley, January 2018

## Graduate Aptitude Tests

CSIR-NET - 2016	(Physics)	: All India Rank 87
GATE - 2017	(Physics)	: All India Rank 162
GRE - 2016	(Physics)	: 990/990
IIT-JAM - 2017	(Physics)	: All India Rank 20
JEST - 2017	(Physics)	: All India Rank 11

## Publications

1. **R. Tom**, T. Rose, I. Bier, H. O'Brien, A. Vazquez-Mayagoitia, and N. Marom. Genarris 2.0: A random structure generator for molecular crystals. (*Submitted*)
2. X. Wang, X. Liu, **R. Tom**, C. Cook, B. Schatschneider, and N. Marom. Phenylated acene derivatives as candidates for intermolecular singlet fission. *The Journal of Physical Chemistry C*, 123(10):5890–5899, 2019
3. **R. Tom** and S. S. Ray. Revisiting the SABRA model: statics and dynamics. *Europhysics Letters*, 120(3):34002, 2017