Rithwik Tom
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Education

Carnegie Mellon University (CMU), Pittsburgh, USA - 15213 August 2017 - Present
Course : Ph.D. (Physics)
Faculty Advisor : Asst. Prof. Noa Marom

Indian Institute of Science (IISc), Bangalore, India - 560012 August 2013 - May 2017
Course : Bachelor of Science (Physics)
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
- Singlet Fission

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++, FORTRAN, MATLAB, Python, Bash.
- Parallel programming paradigms: Shared memory (OpenMP), distributed memory (MPI).
- Debuggers and profilers : GDB, 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

Publications

1. X. Wang, **R. Tom**, X. Liu, D. Congreve, and N. Marom. An energetics perspective on why there are so few triplet-triplet annihilation emitters. *Submitted to Journal of Materials Chemistry C*, 2020
2. X. Liu, **R. Tom**, X. Wang, C. Cook, B. Schatschneider, and N. Marom. Pyrene-stabilized acenes as intermolecular singlet fission candidates: Importance of exciton wave-function convergence. *Journal of Physics: Condensed Matter*, 2020
3. **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. *Computer Physics Communications*, 2020
4. 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
5. **R. Tom** and S. S. Ray. Revisiting the SABRA model: statics and dynamics. *Europhysics Letters*, 120(3):34002, 2017