Rithwik Tom
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Education

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

Course	: Ph.D. (Physics), M.S. (Physics)
Faculty Advisor	: Prof. Noa Marom
Expected Graduation	: May 2022
Thesis	: Prediction of Molecular Crystal Structures

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

Course	: B.S. (Physics)
Faculty Advisors	: Prof. Rahul Pandit and Dr. Samriddhi Shankar Ray
Thesis	: Statistical Properties of Shell Models in Fluid Turbulence

Research Interests

- Electronic Structure Methods
- Molecular Simulation
- High Performance Computing

Research Experience

Crystal Structure Prediction of Molecular Co-crystals *CMU, January 2021 - Present*
Developed and implemented algorithms for predicting structure of molecular co-crystals. Successfully predicted co-crystal structures of previous Cambridge Crystallographic Data Centre (CCDC) blind test targets. *Skills*: C, Python, MPI, MPI4Py, DFT.

Seventh Molecular Crystal Structure Prediction Blind Test *CMU, October 2020 - Present*
International competition organized by CCDC to predict crystal structures of organic molecules.

Optimal Polymorphs of Tetracene for Singlet Fission *CMU, January 2020 - Present*
Discovered polymorphs of tetracene molecule that potentially have an improved singlet fission performance using genetic algorithm based property optimization. *Skills*: Python, MPI4Py, DFT.

Genarris 2.0: Random Crystal Structure Generator *CMU, August 2018 - January 2020*
Developed Genarris 2.0, a random molecular crystal structure generator for seeding crystal structure prediction. Implemented fast algorithms to ensure physical constraints, detect symmetries of molecules and to align them on special positions of space groups. *Skills*: C, Python, MPI, DFT.

Singlet Fission in Acene Derivatives *CMU, May 2018 - December 2019*
Electronic and excitonic properties of phenylated derivatives and pyrene-fused acenes in the gas phase and solid state were investigated using many-body perturbation theory in the GW approximation and Bethe-Salpeter equation (BSE). *Skills*: GW+BSE, DFT.

Solving the Time-Dependent Schrödinger's Equation *NTU, May 2016 - July 2016*
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. *Mentor*: Prof. Yidong Chong. *Skills*: Numerical Methods, MATLAB.

Statistical Properties of Shell Models in Fluid Turbulence *IISc, May 2015 - August 2017*
Simulated shell models to study the energy cascade phenomenon in fluid turbulence. *Skills*: C++, Numerical Methods.

Awards

Molecular Software Sciences Institute Seed Fellowship *January 2021 - June 2021*
Project: Crystal Structure Prediction of Molecular Co-crystals. *Mentor*: Dr. Jonathan Moussa

Rational Solid Form Design Conference Travel Grant *October 2019*

NTU-India Connect Fellowship *May 2016 - July 2016*

KVPY Fellowship *August 2013 - May 2017*

Programming Experience

Code	Role	Language	Purpose
Genarris	Developer	C, Python	Molecular Crystal Structure Prediction
GAtor	Developer	Python	Molecular Crystal Structure Prediction
Arsha	Developer	C++	Chess Engine
ASE	Contributor	Python	Atomic Simulation Environment

Skills

Programming languages	C, C++, Python, MATLAB, Bash, Fortran, Emacs Lisp
Parallel programming paradigms	MPI, OpenMP, OpenACC
Debuggers and profilers	GNU Debugger, GNU Profiler
Testing Frameworks	Ctest, Pytest
Version control system	Git
Electronic structure codes	FHI-aims, Gaussian, Quantum Espresso, BerkeleyGW, DFTB+
Packages/Libraries	ASE, Pymatgen, OpenBabel, Spglib, MPI4Py, Scipy, Scikit-learn, SWIG

Conferences and Workshops

American Physical Society (APS) March Meeting *Online, March 2021*
Presentation: Genarris 2.0: Random Molecular Crystal Structure Generator

MolSSI Workshop on Scientific Software Design for Software Fellows *Online, January 2021*

Rational Solid Form Design and Development Summit *Boston, October 2019*
Poster presentation: Genarris 2.0: Diverse Molecular Crystal Structure Generation by Space Groups

XSEDE HPC Workshop on Message Passing Interface (MPI) *Pittsburgh, September 2019*

Summer School and Workshop on Time Dependent DFT *New Brunswick, August 2019*
Poster presentation: Phenylated Acene Derivatives as Candidates for Intermolecular Singlet Fission

Sixth Annual Workshop on BerkeleyGW *San Francisco, June 2019*
Poster presentation: Phenylated Acene Derivatives as Candidates for Intermolecular Singlet Fission

Recent Developments in Electronic Structure Theory *Urbana-Champaign, May 2019*
Poster presentation: Genarris 2.0: Diverse Molecular Crystal Structure Generation by Space Groups

XSEDE HPC Workshop on OpenACC *Pittsburgh, March 2019*

XSEDE HPC Workshop on OpenMP *Pittsburgh, January 2019*

Fifth Annual Workshop on BerkeleyGW *San Francisco, January 2018*

Publications

1. **R. Tom**, J. Moussa, and N. Marom. Molecular co-crystal prediction using genarris. *(under preparation)*
2. **R. Tom**, S. Gao, and N. Marom. Optimal tetracene polymorphs for singlet fission. *(under preparation)*
3. X. Liu, **R. Tom**, S. Gao, and N. Marom. Assessing zethrene derivatives as singlet fission candidates based on multiple descriptors. *The Journal of Physical Chemistry C*, 124(48):26134–26143, 2020
4. X. Wang, **R. Tom**, X. Liu, D. N. Congreve, and N. Marom. An energetics perspective on why there are so few triplet–triplet annihilation emitters. *Journal of Materials Chemistry C*, 2020
5. **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*, 250:107170, 2020
6. 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
7. 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
8. **R. Tom** and S. S. Ray. Revisiting the SABRA model: statics and dynamics. *Europhysics Letters*, 120(3):34002, 2017