Mohammad Elious Ali Mondal

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Date of Birth	12 December 1998	**Github**	github.com/EliousMondal
Nationality	Indian	**Webpage**	EliousMondal

Education

Ph.D.

2021-now **Ph.D. in Chemistry** at **University of Rochester**
Courses: Quantum Chemistry, Mathematical Methods, Condensed Matter Physics, Statistical Mechanics, Quantum Dynamics, Machine Learning for Molecules, Quantum Optics of Electromagnetic fields, Geometrical Methods in Physics

Bachelors and Masters

2016-2021 **Integrated BS-MS** from **Indian Institute of Science Education and Research, Bhopal**
Major - Chemistry, **CGPA - 8.68/10**
Relevant Courses from Chemistry: Quantum Chemistry, Mathematical Methods, Statistical Mechanics, Molecular Simulations, Molecular Spectroscopy, Group Theory, Chemical Thermodynamics, Organic Chemistry, Biological Chemistry, Photochemistry and Heterocyclic Chemistry.
Relevant Courses from Physics: Condensed Matter Physics, Electronic Structure of Materials.

Research Experience

Sept 2021 - Present **Ph.D. under the supervision of Prof. Pengfei (Frank) Huo (University of Rochester)**

Goal: Quantum dynamics simulations of linear and non-linear spectroscopy for probing mechanisms in Polariton Chemistry

Overview:

1. Developed a code for simulating linear and non-linear spectroscopies for studying quantum dynamics of large complex systems by combining PLDM (Partial linearized density matrix) with Lindblad dynamics for Open Quantum Systems. This can be used to separately treat both Markovian and Non-Markovian effects in the same dynamics simulation.
2. Studying the linear and 2D-ES spectra of Polaritonic systems and using these tools to fundamentally understand the effect of cavity on different dynamical processes in excitonic polaritons.
3. Improvising the current tools to more efficiently simulate spectroscopy and overcoming the approximations of the current PLDM-based method. These include exploring Deep learning trajectory dynamics and more accurate spin-mapping trajectory methods.
4. 2D-IR spectra simulation for understanding the Polariton effects in Vibrational Strong Coupling (VSC).

Skills achieved till now: Path Integral dynamics based on diabatic MMST mapping, Spin-Boson models, Generalised formalism of Linear and Non-Linear Spectroscopy, Open Quantum Systems, Master Equations, Hamiltonians for Cavity QED with molecules.

Aug 2020 - May 2021 **MS-Thesis under the supervision of Dr. Varadharajan Srinivasan (IISER Bhopal)**

Goal: A python code for applying Trajectory-Surface-Hopping (TSH) to study Non-adiabatic processes in Chemistry is to be developed and tested.

Overview: A code for applying decoherence correction to FSSH was developed. I tested the code on some actual molecules and added some features to the already existing code. Some of these features are IDC and EDC correction, fast-NACT calculation based on the orbital overlap, and NAC-vector calculation.

Skills achieved: Learned about non-adiabaticity in chemical processes, HPC computing with python using mpi4py, scientific computing packages(ASE, BSE, Numpy, Scipy), handling NWChem, Newton-X and Turbomole.

May 2019 - July 2019 **Summer Internship under the supervision of Dr. Varadharajan Srinivasan (IISER Bhopal)**

Goal: To study the non-adiabatic effects of an electron placed in double-harmonic well under time-dependent oscillatory perturbations.

Overview: We constructed a model hamiltonian of a double harmonic well (looks like a superposition of two harmonic wells). A time dependent oscillatory perturbation was then applied and the effects of adiabaticity were studied by solving the 1-D Time-Dependent Schrodinger equation using Crank-Nicolson method. Finally, the limits of adiabaticity for this well was determined for this potential.

Skills achieved: Learned about adiabatic effects in Quantum Mechanics, Numerical methods for solving parabolic Partial Differential equations, Scientific computing packages - Numpy,Scipy

June 2018 - July 2018 **Summer Internship under the supervision of Dr. Ayan Datta (IACS Kolkata)**

Goal: Search for possible replacements for A-site cations in organic-Pb-Halide-Perovskites for better moisture stability of solar cells.

Overview: I looked for the Band structures and stability analysis of some organic cations (aromatic,anti-aromatic and homo-aromatic). I was also searching for a possible replacement for the B-Site cation in Perovskites so as to accommodate some bigger A-site organic cations. These were done in a Plane-wave basis DFT code, VASP.

Skills achieved: Handling of Quantum Chemistry Software packages - Gaussian,VASP

Dec 2017 - Jan 2018 **Winter Internship under the supervision of Dr. Nirmal Ganguli (IISER Bhopal)**

Goal: Write a Python code to solve 1-D Schroedinger equation for any 1D-potential.

Overview: I learned some numerical methods to solve eigenvalue problems and in-particular solving 1-D ODEs (Runge-Kutta methods, Numerov method). These methods along with the Shooting method was used to construct a python code for solving the Time-independent Schroedinger equation for any 1-D potential.

Skills achieved Numerical methods for solving eigenvalue equations.

June 2017 - July 2017 **Summer Internship under the supervision of Dr. Nirmal Ganguli (IISER Bhopal)**

Goal: Learn the basics of numerical methods and scientific computing.

Overview: I was exposed to many numerical methods like interpolation, Least-square fitting, Matrix decomposition methods, numerical integration, and differentiation techniques. Using these I wrote a python code to solve Buffon's needle problem and a code to find the percolation probability in 2D lattices.

Skills achieved: Python, Numerical and Scientific computing.

Publications

1. **Quantum Dynamics Simulations of the 2D Spectroscopy of Exciton Polariton**.
   M. Elious Mondal, Eric Koessler, A. Nickolas Vamivakas, Steven T. Cundiff, Todd D. Krauss, Pengfei Huo.
   -***J. Chem. Phys.***
2. **Universal Measure for the Impact of Adiabaticity on Quantum Transitions.**
   R. Pant, P. K. Verma, C. Rangi, **M. Elious Mondal**, M. Bhati, V. Srinivasan, S. Wuster. -***Phys. Rev. Lett***
3. **Theory and Quantum Dynamics Simulations of Exciton-Polariton Motional Narrowing**
   W. Ying, **M. Elious Mondal**, Pengfei Huo. - ***ChemRxiv***
4. **Effects of collective coupling on 2DES of polaritons.**
   M. Elious Mondal, Pengfei Huo. - To be submitted
5. **Efficient 2DES simulation of large polaritonic systems**
   M. Elious Mondal, Pengfei Huo. - To be submitted
6. **Investigating Dissipative Mechanisms in Polariton Transport Via Large-Scale Mixed Quantum-classical Dynamics**
   Benjamin Chng, **M. Elious Mondal**, Pengfei Huo. - To be submitted
7. **Including non-markovian effects in $g^{(2)}$ simulations**
   M. Elious Mondal, Pengfei Huo. - Manuscript under preparation
8. **Stochastic Lindblad dynamics for cavity loss in mapping based trajectory methods.**
   Eric Koessler, **M. Elious Mondal**, Pengfei Huo. - Manuscript under preparation

Conferences and Science outreach

1. Poster presentation at the American Conference on Theoretical Chemistry (ACTC-2024), held at the University of North Carolina, Chapel Hill.
2. Poster presentation at the Wintern school on Quantum Information for Chemistry (2024), held at University of California, Los Angeles
3. Poster presentation at the Graduate Research symposium 2024 at University of Rochester
4. Poster presentation at Gordon Research Conference - Light Matter Interactions 2023, held at Salve Regina University, Rhode Island
5. Poster presentation at Telluride School for Theoretical Chemistry 2023 held at Telluride Science
6. Poster presentation at TDDFT workshop 2023 held at Rutgers University, newark
7. Poster presentation at TDDFT Summer School 2023 held at Rutgers University, newark
8. ACS-NERM 2022 regional conference held at Rochester
9. Huo-group science outreach for High school students, 2022, University of Rochester
10. ACS-MARM 2022 regional conference held at TCNJ (The College of New Jersey), Trenton
11. National Science (VIJYOSHI) Camp, 2016, held at IISER-Kolkata

Teaching

1. **CHM 451 (Fall 2023):** Teaching Assistant for Quantum Chemistry
2. **Science Outreach (Summer 2023):** Journey to Molecular World - a short summer course for K-12 students aimed as a brief introduction to Theoretical and Computational Chemistry
3. **CHM 451 (Fall 2022):** Teaching Assistant for Quantum Chemistry

4. **CHM 251(/441) (Fall 2022):** Teaching Assistant for Physical Chemistry - I
5. **Science Outreach (Summer 2022):** Journey to Molecular World - a short summer course for K-12 students aimed as a brief introduction to Theoretical and Computational Chemistry
6. **CHM 132 (Spring 2022):** Teaching Assistant for General Chemistry - II laboratory
7. **CHM 131 (Fall 2021):** Teaching Assistant for General Chemistry - I laboratory

Computational Skills

1. **Programming Languages:** Python, C++, Julia, LaTeX, Git
2. **Libraries & Tools:** Numpy, Scipy, Numba, QuTip, Cython, Matplotlib, PySCF, ASE
3. **Computing/HPC:** mpi4py, Command-line(Linux), Bash
4. **Softwares:** INQ, NWChem, Newton-X, Turbomole, Gaussian, Avogadro

Awards an Achievements

1. **The Journal of Physical Chemistry poster award** at the American Conference on Theoretical Chemistry, (ACTC-2024).
2. **Wu Fellowship (2023)** by Department of Chemistry, University of Rochester. Selected by the faculty on the basis of outstanding research support in chemistry
3. **Kishore Vaigyanik Protsahan Yojana (KVPY) fellowship (2016-2021)** by Department of Science ad Technology(DST) - India, to pursue a career in Fundamental Sciences.
4. **Certificate of Merit** by AISSCE (Higher Seccondary examination of CBSE)

Positions of Responsibility

1. **Undergraduate Research Mentor** of Rittik Mandal, an i-Scholar at the Department of Chemistry, the University of Rochester for Summer 2024.
2. **Undergraduate Research Mentor** of o Abobakar Sediq Miakhel, an undergraduate student at the Department of Physics, the University of Rochester. He will be an undergraduate researcher at the Huo lab for the academic year 2024-2025.
3. **Graduate Mentor** of Jhoan Fernandez Sanchez, an incoming graduate student at the Department of Chemistry, the University of Rochester for Fall 2024.
4. **Graduate Mentor** of Sanchari Sannigrahi, an incoming graduate student at the Department of Chemistry, the University of Rochester for Fall 2023.
5. **Graduate Mentor** of Sebastian Montillo, an incoming graduate student at the Department of Chemistry, the University of Rochester for Fall 2022.
6. **Taekwondo Coordinator** of IISER Bhopal from May, 2017 to May, 2019
7. **Mess-President at IISER Bhopal** from February, 2020 to October, 2020