Mohammad Elious Ali Mondal

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Date of Birth	12 December 1998	**Github**	github.com/EliousMondal
Nationality	Indian	**Google Scholar**	M. Elious Mondal

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-Electronic 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. Efficient simulations of quantum dynamics of large polaritonic systems for predicting spectroscopic and transport properties.

Skills achieved till now: Path Integral dynamics based on diabatic MMST mapping, Spin-Boson models, Generalised formalism of Linear and Non-Linear Spectroscopy, 2DES, 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.

Publications

1. **Quantum Dynamics Simulations of the 2D Spectroscopy of Exciton Polariton**.
   M. E. Mondal, E. Koessler, A. N. Vamivakas, S. T. Cundiff, T. D. Krauss, Pengfei Huo.
   -***J. Chem. Phys., 159, 094102 (2023)***
2. **Universal Measure for the Impact of Adiabaticity on Quantum Transitions.**
   R. Pant, P. K. Verma, C. Rangi, **M. E. Mondal**, M. Bhati, V. Srinivasan, S. Wuster. -***Phys. Rev. Lett, 132 (12), 11 (2024)***
3. **Theory and Quantum Dynamics Simulations of Exciton-Polariton Motional Narrowing**
   W. Ying, **M. E. Mondal**, P. Huo. - ***J. Chem. Phys., 161, 064105 (2024)***
4. **Polariton Spectra under the Collective Coupling Regime. I. Efficient Simulation of Linear Spectra**
   M. E. Mondal, A. N. Vamivakas, S. T. Cundiff, T. D. Krauss, P. Huo. - ***J. Chem. Phys., 162, 014114 (2025)***
5. **Quantum Dynamics Simulations of the Polariton Transport**
   B. Chng, **M. E. Mondal**, W. Ying, P. Huo. - ***NanoLetters (2025)***
6. **Polariton Spectra under the Collective Coupling Regime. II. Efficient Simulation of 2DES Spectra**
   M. E. Mondal, A. N. Vamivakas, S. T. Cundiff, T. D. Krauss, P. Huo. - ***ChemRxiv*** - Accepted in ***J. Chem. Phys.***
7. **Polaron Decoupling Effect Leading to Long-Lived Polaritonic Coherence.**
   M. E. Mondal, A. N. Vamivakas, S. T. Cundiff, T. D. Krauss, P. Huo. - To be submitted
8. **Including non-markovian effects in $g^{(2)}$ simulations**
   M. E. Mondal, P. Huo. - Manuscript under preparation

Presentations and Talks

1. **American Conference on Theoretical Chemistry (ACTC-2024)**, University of North Carolina, Chapel Hill, *"Efficient simulation of collective effects in spectroscopy of exciton-polaritons"* - **Poster**
2. **Winter school on Quantum Information for Chemistry (2024)**, University of California, Los Angeles, *"Quantum Dynamics Simulations of Polariton Spectroscopy"* - **Poster & Talk**
3. **Graduate Research Symposium 2024**, University of Rochester, *"Quantum Dynamics Simulations of Polariton Spectroscopy"* - **Poster**
4. **Gordon Research Conference - Light Matter Interactions 2023**, Salve Regina University, Rhode Island, *"Quantum Dynamics Simulations of the 2D Spectroscpy of Exciton Polaritons"* - **Poster**
5. **Telluride School for Theoretical Chemistry 2023, Telluride Science**, *"Quantum Dynamics Simulations of the 2D Spectroscpy of Exciton Polaritons"* - **Poster**
6. **TDDFT workshop 2023**, Rutgers University, Newark, *"Quantum Dynamics Simulations of the 2D Spectroscpy of Exciton Polaritons"* - **Poster**

7. **TDDFT Summer School 2023**, Rutgers University, Newark, *"Quantum Dynamics Simulations of the 2D Spectroscpy of Exciton Polaritons"* - **Poster**
8. **ACS Spring 2023**, Indiana Convention Center, Indianapolis
9. **ACS-NERM 2022 regional conference**, Rochester Convention Center
10. **ACS-MARM 2022 regional conference**, The College of New Jersey (TCNJ), Trenton
11. **National Science (VIJYOSHI) Camp, 2016**, 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++, Cython, Julia, LaTeX, Git
2. **Libraries & Tools:** Eigen, Numpy, Scipy, Numba, PyTorch, CuPy, QuTip, Pandas, Matplotlib, ASE
3. **Computing/HPC:** open-mpi, mpi4py, Command-line(Linux), Bash
4. **Softwares:** INQ, NWChem, Newton-X, Turbomole, Gaussian, Avogadro, PySCF

Awards an Achievements

1. **Wu Fellowship (2024)** by Department of Chemistry, University of Rochester. Selected by the faculty on the basis of outstanding research support in chemistry
2. **The Journal of Physical Chemistry poster award** at the American Conference on Theoretical Chemistry, (**ACTC-2024**).
3. **Wu Fellowship (2023)** by Department of Chemistry, University of Rochester. Selected by the faculty on the basis of outstanding research support in chemistry
4. **Kishore Vaigyanik Protsahan Yojana (KVPY) fellowship (2016-2021)** by Department of Science ad Technology (DST) - India, to pursue a career in Fundamental Sciences.
5. **Certificate of Merit (AISSCE 2015)**, Higher Secondary 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 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