Mohammad Elious Ali Mondal

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		Email	mmondal@ur.rochester.edu
Date of Birth	12 December 1998	**Github**	github.com/EliousMondal
		Google Scholar	M. Elious Mondal

Education

Ph.D.

2021-now **Ph.D. in Chemistry**, **University of Rochester**
Courses: Geometrical Methods in Physics, Quantum Optics of Electromagnetic fields.

Masters

2021-2023 **MS in Chemistry**, **University of Rochester**
Courses: Quantum Chemistry, Mathematical Methods, Condensed Matter Physics, Statistical Mechanics, Quantum Dynamics, Machine Learning for Molecules.

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,
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)**

Overview:

1. Developed software to simulate linear and nonlinear 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. Developed efficient and accurate strategies to reduce the computational cost of linear and nonlinear spectroscopy for large polaritonic systems for any general Mixed Quantum Classical (MQC) dynamics method.
3. Improving current tools to simulate spectroscopy more efficiently 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 acquired: Path Integral MQC dynamics, Mapping formalisms, Spin-Boson models, Generalised formalism of Linear and Non-Linear Spectroscopy, Open Quantum Systems, Master Equations, Cavity QED Hamiltonians, Analog Simulations, LSTM and RNN's.

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

Overview: A code for applying decoherence correction to FSSH was developed. I benchmarked the code by performing population dynamics of Ethylene and N_2, and added some features to the already existing code. Some of these features are IDC and EDC (Decoherence) corrections, fast-NACT calculation based on the orbital overlap, and NAC-vector calculation.

Skills aquired: 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. *Long-Lived Polaritonic Coherence and Polaron Decoupling Effects in 2D Electronic Spectra.*
M. E. Mondal, S. Park, M. Son, A. N. Vamivakas, S. T. Cundiff, T. D. Krauss, P. Huo. - ***ChemRxiv***

2. *Vibrational Strong Coupling in Cavity QED forms a Macroscopic Quantum State*
M. E. Mondal, S. M. Vega, P. Huo. - ***ChemRxiv***

3. *Collective Effects in Polariton Chemistry and Photophysics*
W. Ying, **M. E. Mondal**, E. R. Koessler, S. M. Vega, P. Huo. - Accepted in ***Ann. Rev. Phys. Chem.***

4. *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. - ***J. Chem. Phys. 162 (7), 074110 (2025)***

5. *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)***

6. *Quantum Dynamics Simulations of the Polariton Transport*
B. Chng, **M. E. Mondal**, W. Ying, P. Huo. - ***Nano Letters 25 (4), 1617-1622 (2025)***

7. *Theory and Quantum Dynamics Simulations of Exciton-Polariton Motional Narrowing*
W. Ying, **M. E. Mondal**, P. Huo. - ***J. Chem. Phys., 161, 064105 (2024)***

8. *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)***

9. *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)***

Publications in Preparation

1. *Normal Incidence Condition in Vibrational Strong Coupling for Macroscopic Condensation*
M. E. Mondal, S. M. Vega, P. Huo. - To be submitted

2. *Molecular disorder preserves motional narrowing in exciton polaritons*
M. E. Mondal, W. Ying, P. Huo. - To be submitted

3. *Dynamical low rank propagation of higher excitation manifolds in exciton polaritons*
M. E. Mondal, P. Huo. - Under preparation

4. *Spectroscopy of exciton polaritons with Classical Path Approximation*
M. E. Mondal, B. Chng, B. M. Weight, W. Ying, S. M. Vega, P. Huo. - To be submitted

5. *Efficient computation of ab initio polaritonic spectra with Classical Path dynamics*
M. E. Mondal, B. Chng, B. M. Weight, P. Huo. - Under preparation

6. *Ab initio Polariton Transport dynamics with Classical Path Approximation*
   B. Chng, B. M. Weight, **M. E. Mondal**, P. Huo. - To be submitted
7. *Polaron transformed Ehrenfest dynamics for high frequency phonon modes*
   M. E. Mondal, S. M. Vega, P. Huo. - To be submitted
8. *Predicting linear spectra from classical path trajectories*
   A. S. Miakhel, **M. E. Mondal**, S. M. Vega, P. Huo. - To be submitted (Equal first author)
9. *Effective longitudinal coupling in superconducting qubits via two resonators*
   M. E. Mondal, M. A. Ijaz, M. S. Blok, P. Huo. - Under preparation
10. *Analog simulations of Markus inversion*
    M. A. Ijaz, **M. E. Mondal**, M. S. Blok, P. Huo. - Under preparation (Equal first author)

Presentations and Talks

1. **American Chemical Society Spring 2025**, Anaheim Convention Center, Anaheim, California, *"Exploring Dissipative Effects in Molecular Exciton-Polariton Transport"* - **Talk**
2. **American Physical Society March Meetings 2025**, Anaheim Convention Center, Anaheim, California, *"Exploring Dissipative Effects in Molecular Exciton-Polariton Transport"* - **Talk**
3. **American Physical Society March Meetings 2025**, Anaheim Convention Center, Anaheim, California, *"Efficient Simulation of Polariton Spectra under the Collective Coupling"* - **Talk & Poster**
4. **American Conference on Theoretical Chemistry 2024**, University of North Carolina, Chapel Hill, *"Efficient simulation of collective effects in spectroscopy of exciton-polaritons"* - **Poster**
5. **Winter school on Quantum Information for Chemistry (2024)**, University of California, Los Angeles, *"Quantum Dynamics Simulations of Polariton Spectroscopy"* - **Poster & Talk**
6. **Graduate Research Symposium 2024**, University of Rochester, *"Quantum Dynamics Simulations of Polariton Spectroscopy"* - **Poster**
7. **Gordon Research Conference - Light Matter Interactions 2023**, Salve Regina University, Rhode Island, *"Quantum Dynamics Simulations of the 2D Spectroscopy of Exciton Polaritons"* - **Poster**
8. **Telluride School for Theoretical Chemistry 2023, Telluride Science**, *"Quantum Dynamics Simulations of the 2D Spectroscopy of Exciton Polaritons"* - **Poster**
9. **TDDFT workshop 2023**, Rutgers University, Newark, *"Quantum Dynamics Simulations of the 2D Spectroscopy of Exciton Polaritons"* - **Poster**
10. **TDDFT Summer School 2023**, Rutgers University, Newark, *"Quantum Dynamics Simulations of the 2D Spectroscopy of Exciton Polaritons"* - **Poster**

Teaching

1. **CHM 451 (Fall 2023):** Teaching Assistant for Quantum Chemistry (Graduate level course)
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 (Graduate level course)
4. **CHM 251(/441) (Fall 2022):** Teaching Assistant for Physical Chemistry - I (Undergraduate level course)
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 (Undergraduate level course)

Computational Skills

1. **Programming Languages:** Python, C++, Cython, Julia, LaTeX, Git
2. **Libraries & Packages:** Eigen, Numpy, Scipy, Numba, PyTorch, CuPy, QuTip, Pandas, Matplotlib
3. **HPC & Parallelization:** open-mpi, mpi4py, Command-line(Linux), Bash
4. **Quantum Chemistry Software:** NWChem, Newton-X, Turbomole, Gaussian, Avogadro, PySCF, INQ

Awards and Achievements

1. Finalist of **ACS Physical Chemistry Graduate Awards (2025)** in Theoretical Chemistry
2. **Agnes M. and George Messersmith Fellowship (2025)** It is one of the University's most competitive dissertation fellowships and is given to students who display exceptional ability and promise.
3. **Wu Fellowship (2024)** by the Department of Chemistry, University of Rochester. Selected by the Chemistry faculty committee on the basis of outstanding research support in chemistry.
4. **The Journal of Physical Chemistry poster award** at the American Conference on Theoretical Chemistry (**ACTC-2024**).
5. **Wu Fellowship (2023)** by the Department of Chemistry, University of Rochester. Selected by the Chemistry faculty committee on the basis of outstanding research support in chemistry.
6. **Kishore Vaigyanik Protsahan Yojana (KVPY) fellowship (2016-2021)** by the Department of Science and Technology (DST) - India, to pursue a career in Fundamental Sciences.
7. **Certificate of Merit (AISSCE 2015)**, Higher Secondary examination of CBSE.

Positions of Responsibility

1. **Graduate Research Mentor** of Hsien-Chao Jan, a first-year theory graduate student in the Department of Chemistry at the University of Rochester.
2. **Undergraduate Research Mentor** of Zhenyi Lin, an undergraduate in the Department of Chemistry at the University of Rochester for the academic year 2025-2026.
3. **Undergraduate Research Mentor** of Abobakar Sediq Miakhel, an undergraduate student in the Department of Physics at the University of Rochester for the academic year 2025-2026.
4. **Undergraduate Research Mentor** of Rittik Mandal, an i-Scholar in the Department of Chemistry at the University of Rochester for Summer 2024.
5. **Graduate Mentor** of Jhoan Fernandez Sanchez, an incoming graduate student in the Department of Chemistry at the University of Rochester for Fall 2024.
6. **Graduate (Research) Mentor** of Sanchari Sannigrahi, an incoming graduate student in the Department of Chemistry at the University of Rochester for Fall 2023.
7. **Graduate Mentor** of Sebastian Montillo, an incoming graduate student in the Department of Chemistry at the University of Rochester for Fall 2022.

Referees for recommendation letters

1. **Prof. Pengfei (Frank) Huo** - Department of Chemistry, University of Rochester
   Email: pengfei.huo@rochester.edu
2. **Prof. David W. McCamant** - Department of Chemistry, University of Rochester
   Email: david.mccamant@rochester.edu
3. **Prof. Todd D. Krauss** - Department of Chemistry, University of Rochester
   Email: todd.krauss@rochester.edu