**Last Name: Mondal First Name: Mohammad Elious Ali**

**Advisor: Pengfei (Frank) Huo Date: 07 / 08 / 2023**

**Year Entered PhD Program: 2022 Years Completed in Program: 2.5**

**Number of Course Credits Completed: 29 Cumulative GPA: 3.448**

**Target Graduation Date: 08 / 31 / 2026**

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| --- | --- | --- | --- |
| **Program Requirement** | **Completed (Date)** | **Scheduled (Date)** | **Overdue** |
| Cumulative Exams | **02 / 11 / 22, 03 / 11 / 22, 04 / 08 / 22, 05 / 13 / 22, 06 / 10 / 22, 07 / 08 / 22** |  |  |
| Second Year Oral Exam | **06 / 12 / 2023** |  |  |
| Third Year Seminar | **03 / 11 / 2024** |  |  |
| Fourth Year Review |  |  |  |

**1. Fellowships, Travel Grants, and Awards**

1. Applied for (include application date)

* Department of Chemistry Travel Award (2023)
* Department fellowship (2023)
* Telluride School on Theoretical Chemistry (2023)
* MOLSSI software fellowship (2023)
* Hooker Fellowship (2024)
* Goodman fellowship (2024)
* Winter School on Quantum Information Science for Chemistry (2024)
* MOLSSI software fellowship (2024)
* Department of Chemistry Travel Award (2024)

1. Received (include Departmental and University Teaching Awards AND include any fellowships, travel grants, and awards received in previous years)

* Wu Fellowship (2023 - 2024)
* Telluride School on Theoretical Chemistry (2023)
* Winter School on Quantum Information Science for Chemistry (2024)
* Journal of Chemical Physics Poster Award at ACTC (2024)

**2. Synergistic Activities and Departmental/University Service**

1. List any teaching activities, including teaching assistant positions (with course number and instructor) and any mentoring activities (name and time period for research mentorship responsibilities for undergraduate, first-year graduate, or high school research students)

* General Chemistry I
  + Course Number: CHEM131, FALL2021ASE
  + Instructor: Prof. Courtney Stanford
* General Chemistry II
  + Course Number: CHEM132, SPRING2022ASE
  + Instructor: Prof. Courtney Stanford
* Physical Chemistry I
  + Course Number: CHEM251, Fall 2022
  + Instructor: Prof. Todd D. Krauss
* Quantum Chemistry I
  + Course Number: CHEM451, Fall 2022
  + Instructor: Prof. Pengfei (Frank) Huo
* Quantum Chemistry I
  + Course Number: CHEM451, Fall 2023
  + Instructor: Prof. Pengfei (Frank) Huo
* Graduate Research mentoring
  + Sebastian Montillo Vega (Chemistry 2022)
  + Sanchari Sannigrahi (Chemistry 2024)
  + Jhoan Fernandez Sanchez (Chemistry 2025)
* Undergraduate Research mentoring
  + Rittik Mandal (I-scholar 2024)
  + Abobakar Sediq Miakhel (Physics Undergraduate researcher, 2024)

1. List any other synergistic or outreach activities that are relevant to your graduate studies in chemistry (include outreach, departmental or university committee service, and volunteer efforts)

* Upward Bound outreach from Huo Group, 07/25/2022
* Upward Bound outreach from Huo Group, 07/26/2023

**3. Publications since entering the PhD program**

1. Published (please provide a complete reference, including all papers published while a student at the University of Rochester)

* Quantum Dynamics Simulations of the 2D spectroscopy for Exciton Polaritons.
  + Authors: **M. E. Mondal**, E. Koessler, J. Provazza, A. N. Vamivakas, S. Cundiff, T. D. Krauss, P. Huo.
  + Journal: Journal of Chemical Physics
  + Publication date: 09 / 01 / 2023
* Universal Measure for the Impact of Adiabaticity on Quantum Transitions.
  + Authors: R. Pant, P. K. Verma, C. Rangi, **M. E. Mondal**, M. Bhati, V. Srinivasan, S. Wuster
  + Journal: Physical Review Letters
  + Publication date: 03 / 22 / 2024

1. Submitted (please include authors, title, journal to which submitted, and submission date; do NOT include manuscripts “in preparation”)

* Theory and Quantum Dynamics Simulations of Exciton-Polariton Motional Narrowing
  + Authors: Wenxiang Ying, **M. Elious Mondal**, P. Huo
  + Journal: ChemRxiv (Submitted to Journal of Chemical Physics)
  + Submission date: 06 / 06 / 2024

**4. Presentations at regional/national/international conferences**

(Include conference name, location, date, presentation type (poster/talk), and title; include all conferences attended while a student at the University of Rochester)

* Summer School: TDDFT Summer School 2023
  + Location: University of Rutgers, Newark
  + Presentation type: Poster
  + Title: “Quantum Dynamics simulations for 2D spectroscopy for exciton Polaritons”
* Summer School: Telluride School on Theoretical Chemistry 2023
  + Location: Telluride
  + Presentation type: Poster
  + Title: “Quantum Dynamics simulations for 2D spectroscopy for exciton Polaritons”
* Conference: Gordon Research Conference (GRC) on light-matter interactions 2023
  + Location: Salve Regina University, Rhode Island
  + Presentation type: Poster
  + Title: “Quantum Dynamics simulations for 2D spectroscopy for exciton Polaritons”
* Winter School: Quantum Information Science for Chemistry (2024)
  + Location: University of California, Los Angeles
  + Presentation type: Poster
  + Title: “Quantum Dynamics simulations for 2D spectroscopy for exciton Polaritons”
* Symposium: Graduate Research Symposium (AS&E) 2024
  + Location: University of Rochester
  + Presentation type: Poster
  + Title: “Quantum Dynamics simulations for 2D spectroscopy for exciton Polaritons”
* Conference: American Conference on Theoretical Chemistry (ACTC) 2024
  + Location: University of North Carolina (UNC), Chapel Hill.
  + Presentation type: Poster.
  + Title: “Efficient Simulation of Collective Effects in Spectroscopy of exciton-polaritons”.
  + Award: Journal of Chemical Physics Poster Award

**5. Research Accomplishments**

Briefly (limit 1000 words) describe significant research accomplishments in the last year.

Second year students should attach their second year proposal document to the end of this document and in this section write, “See attached second year proposal.”

The strong coupling of molecular excitations with a quantized radiation field inside a confined optical cavity produces a set of light-matter hybrid states known as polaritons. Recent experiments have shown that these polariton states have great promise in changing the reactivities of molecules and effectively reducing the coupling between excitons and phonons, commonly called the polaron decoupling effect. This polaron decoupling effect results in an enhanced charge transfer rate constant, a reduction of the homogeneous linewidth of spectra, and causes ballistic exciton–polariton transport. In particular, the exciton-polariton coherence lifetime can be prolonged due to reduced coupling with the phonon bath. 2D electronic spectroscopy is one of the most powerful experimental techniques to directly probe polaron decoupling and coherence enhancement. Although a powerful technique, the spectra can be very difficult to interpret because of the congested signals produced by condensed phase systems. To better understand the experiments, we come up with efficient tools to accurately simulate linear and non-linear spectroscopy of exciton-polaritons. The major advances in the project in the last year are

* We developed a mixed-quantum classical formalism (Lindblad + Partial Linearized Density Matrix, L-PLDM) to simulate the linear and non-linear spectroscopy of exciton-polaritons. The formalism allows us to combine Markovian and non-Markovian dynamics of cavity and molecule degrees of freedom and we can very generally use this to simulate other kinds of systems (other than polaritons) where we can assign different degree of markovinity for different parts of our system. Also, the algorithm can be very straightforwardly extended to include higher-dimensional spectroscopy experiments.
* Simulating non-linear spectroscopy becomes exponentially expensive with the increase in the size of the system as describing the dynamics needs the inclusion of 2nd excitation manifold to describe Excited state absorption pathways. Specifically for exciton-polariton systems with N-molecules in the presence of a cavity mode, the second excited space increases as ***O(N2),*** and the Hilbert space expands as ***O(N4)***. A reduced system dynamics involves computation expense of order ***O(N6)***. We use the symmetry and sparsity of the polaritonic Hamiltonian, and the forward-backward nature of L-PLDM to reduce the computational cost to ***O(N2).*** Furthermore, simulating 2D spectroscopy itself is expensive over the length of simulation and scales as ***O(T3)*** for a laser of time length ***T***. We further come up with a vectorization strategy to efficiently control this cost to ***O(1).***
* We use our efficient formalism to compute the spectroscopy of exciton-polaritons
  + We study the linear spectra lineshapes of the exciton-polaritons under various energetic and orientational disorders of very large systems (1000 – 10000 molecules). We observe the disappearance of strong coupling effects with the increasing disorder as a broadening of lineshapes and a decrease in absorption intensity. The orientation disorder, on the other hand, does not affect the linewidth but reduces the effective Rabi-splitting.
  + We further simulate the 2D spectroscopy of exciton-polaritons for different N. We reproduce the experimental lineshape slope tilt phenomena for polaron decoupling of polaritons. We observe that the lineshape is mostly dominated by non-rephasing signals for systems with higher N suggesting a shift in the energy transfer pathway with increasing N. We further demonstrate the enhancement of polaritonic coherences due to an increase of the number of molecules coupled to the cavity.

**6. Research Goals**

1. Briefly describe (limit 500 words) your **short-term** research goals for the next year (including project objectives, manuscript preparation and submission, etc.). Second year students write, “See attached second year proposal” and attach the research summary and proposal to the end of this document.

In the short term, I want to expand the capabilities of present formalism.

* On the theory side, I would like to explore the possibility of using methods like GQME (Generalized Quantum Master Equation) and Transfer tensor methods to improve the accuracy and also reduce the computational cost.
* On the computation side, I would like to incorporate the use of GPU for better usage of my vectorized algorithm and further push the limit of the present simulation capability to study bigger systems.
* On the applications side, there have been a lot of recent 2D spectra experiments demonstrating the enhancement of photophysical properties in various exciton-polaritonic systems. I would like to use my method to try to simulate and understand the underlying physics of those experiments.

1. Briefly describe your **long-term** research goals (limit 750 words) for your project beyond the next year (including project objectives, manuscript preparation and submission, etc.).

For the long-term goal, my broader aim is to learn different aspects of quantum dynamics theory and simulations for general systems beyond Polaritons.

* From the theory perspective
  + My current research methodology almost only revolves around a specific semiclassical method, PLDM. Although it is a good method for condensed phase dynamics, it does not perform optimally for a huge class of system-bath models. Also, if we look at structured environments with a very strong coupling between system and bath degrees of freedom (bath with very structured spectral density), almost all the semiclassical methods break down. So, one of my major long-term goals is to learn other approximate dynamics methods or methods that assume formalisms other than semi-classics like Master equations, tensor trains, etc.
  + Learning approximate methods is insightful but each method comes with its own flavor of approximations. Thus, no approximate method can describe all the physics of a specific chemical dynamics problem. Thus it becomes a necessity to have a general idea about what an exact dynamics looks like. There are a lot of exact dynamics methods that are fairly cheap for smaller models and can give a lot of intuition for what approximations should be done to get correct dynamics for larger systems using a semiclassical method. Thus I also plan to explore the different exact dynamics methods (HEOM, MCTDH, TD-DMRG) and learn their proper usage.
  + Along with learning the existing tools for simulating quantum dynamics, I also plan to explore the field of developing new dynamics methods for different classes of problems. Similar to the symmetry in the Hamiltonian in my current project, I was able to use it to come up with an efficient scheme for simulating correlation functions, I plan to look into developing methods that reduce the computational cost of the current state-of-the-art.
  + I also want to explore the area of quantum chemistry. Within the chemistry community, this field is way more developed than quantum dynamics. There already exists a lot of formalisms and algorithms for efficient and accurate simulations of large systems. I would like to learn the techniques of quantum chemistry and use those from a dynamics perspective.
* From the perspective of the application of the theory
  + I plan to explore more about polaritons and keep exploring the collective effects in different realistic regimes. A similar kind of Hamiltonian form is also assumed in a lot of condensed matter systems and applying our methods to study the exotic physics of those will be enlightening.
  + The spectroscopic measurements are direct probes of correlation between different observables of our subsystem and so I plan to learn about other forms of spectroscopy experiments and study them from a dynamics perspective.

**7. Career Planning Goals**

1. Briefly (limit 500 words) describe your specific **short-term** career development goals (including talking with seminar speakers, identifying possible postdoctoral research advisors, or exploring career options).

* I have explored a few conferences till now and learned a lot from them. I plan to attend more conferences related to my research in the future and keep making more academic connections along the way
* I have also attended a few summer and winter schools on different topics and this helped me learn about other possible research directions and applications of my current research. I will try to attend a few more schools in some other areas like Electronic structure, Machine Learning, High-performance Computing, and Quantum Computation. These will help me broaden my knowledge and expertise.
* Internships are a great way of learning about things not directly related to my research and also make some future connections for post-doctoral positions. I plan to look for some academic research internships in some universities or national labs to help me decide about my future academic research direction.

1. Briefly (limit 500 words) describe your specific **long-term** career development goals (including application for jobs or postdoctoral research positions).

* I plan to take the academic path. So I will be pursuing my post-doctoral research in the near future. After that, I plan to apply for a professorship and establish my research own group.

**8. Safety**

**A.** If you work in a research lab, list the five most dangerous procedures you do.

**B.** Review the Standard Operating Procedures (SOPs) for these five topics on the Chemistry Department Safety Wiki. Remember that you can also utilize SOPs written by other research groups.

If any topic is missing write a SOP for that topic. Attach your new SOP and send a copy to Tessa Baker (tbaker10@ur.rochester.edu).

If all five topics exist review the SOPs and resign that you have read the five SOPs. Send an e-mail Tessa once complete so she can forward the list to your committee members.

During your review of SOPs, comment if you do anything differently than the SOP states and why you think your procedure is safer or more appropriate. Also list any corrections you think should be made to the SOP.

**Please attach your updated CV to this report.**

**Scheduled Date for Annual Review Meeting: 11 / 03 / 2024**

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Student’s Signature

**Committee Approval of Student Progress (Note: First-year students only require the signature of their research advisor):**

**\_\_\_\_\_\_**Todd D. Krauss**\_\_\_\_\_\_\_\_\_\_\_\_\_\_ \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_**

Advisor’s NameAdvisor’s Signature

**\_\_\_\_\_\_\_**David W. McCamant**\_\_\_\_\_\_\_\_\_ \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_**

Advisor’s NameAdvisor’s Signature

**\_\_\_\_\_\_\_**Pengfei (Frank) Huo**\_\_\_\_\_\_\_\_\_ \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_**

Advisor’s NameAdvisor’s Signature