CCQ Spring 2023 Predoctoral Research Program Projects

CCQ expects to offer several predoctoral research positions for the winter/spring of 2023. The aim of this Predoctoral Program is to provide graduate students pursuing their PhD in a relevant field the opportunity to be employed at the CCQ for the purpose of working on a research project with one or more CCQ staff mentors. An application for an predoctoral position should include a statement of a preferred faculty supervisor and of preferred project.

Here is a list of potential projects for spring 2023 Predoctoral Research Program at CCQ. If you would like more information, please contact one of the scientists involved. *Predoctoral candidates may also propose projects of their own or in consultation with other CCQ staff.*

Efficient numerical methods for the nonequilibrium Dyson equation
Contact- Jason Kaye (jkaye@flatironinstitute.org)

The use of the Keldysh approach in the simulation of quantum many-body dynamics out of equilibrium has grown in popularity over the last several years. This strategy requires solving a collection of nonlinear Volterra integro-differential equations, referred to as the nonequilibrium Dyson equations (NDE), for the various Keldysh components of the many-body Green's function. One of the primary computational bottlenecks in solving the NDE is the presence of memory, or history integrals, which leads to a naive cubic scaling with the number of time steps. This limits practical simulations to short times, and represents a significant limitation of the Keldysh method. However, recent efforts involving linear algebraic compression methods have led to a reduced scaling for a wide class of problems. This project will aim to continue this work, by investigating improved compression algorithms, alternative formulations of the NDE, high-order adaptive time stepping methods, and/or parallelization strategies. The project will focus primarily on algorithm development, and would therefore be a good fit for an individual with a strong interest in numerical methods for scientific computing, and applied mathematics.

References

1. J. Kaye, D. Golez. "Low rank compression in the numerical solution of the nonequilibrium Dyson equation," SciPost Phys. 10, 091 (2021).
2. M. Schuler, D. Golez, Y. Murakami, N. Bittner, A. Herrmann, H. U. R. Strand, P. Werner, M. Eckstein. "NESSi: The Non-Equilibrium Systems Simulation package," Comput. Phys. Commun. 257, 107484 (2020).
3. F. Meirinhos, M. Kajan, J. Kroha, T. Bode. "Adaptive numerical solution of Kadanoff-Baym equations," SciPost Phys. Core 5, 030 (2022).

Strong light-matter coupling in molecular systems
Contact: Johannes Flick (jflick@flatironinstitute.org

Strong light-matter interactions in optical cavities or nanoplasmonic systems can now be used to alter chemical reactions or materials properties. To understand these processes where light and matter both have to be treated quantum mechanically, our work includes method development on suitable computational methods for this regime as well as their applications to problems in the field. In the following we outline possible research projects for graduate students interested in the CCQ predoc program. We also welcome your own ideas for research projects.

I) Cavity effects on ground state chemical reactions
Experimental results in the collective strong light-matter coupling regime have successfully demonstrated the ability to alter chemical reactions. On the other hand, recent realization of nanoplasmonic systems have demonstrated the strong coupling regime on the level of single molecular strong coupling. In this project, we explore from first principles using quantum-electrodynamical density-functional theory [1] and polaritonic coupled cluster methods [2] how chemical landscapes can be changed under single molecule strong light-matter coupling by considering photonic correlations and dissipation effects. This project will make you familiar with high-performance computing systems, the electronic structure software, and theoretical concepts for chemical reactions.

1. J. Flick, Simple Exchange-Correlation Energy Functionals for Strongly Coupled Light-Matter Systems based on the Fluctuation-Dissipation Theorem, Phys. Rev. Lett. (2022).
2. F Pavošević, S Hammes-Schiffer, A Rubio, Cavity-Modulated Proton Transfer Reactions, J Flick, J. Am. Chem. Soc. 2022, 144, 11, 4995–5002.

II) Characterization of the strong coupling of molecular plasmons
The classification of electronic excitations in molecules and molecular nanostructures plays an important role when tailoring materials with desired properties. One example are plasmons, which typically appear in large solid-state systems as density oscillations. In molecular systems, molecular plasmons living on few atoms can be used for the active nanoscale manipulation of visible light. In this project we will explore the strong light-matter coupling of molecular plasmons with chemical degrees of freedom using linear-response density-functional theory for QED systems. This project will make you familiar with high-performance computing systems, ab-initio electronic structure software and the python software language.

1. Bernadotte S., Evers F., Jacob, C. R. (2013) Plasmons in Molecules, J. Phys. Chem. C 2013, 117, 4, 1863–1878.
2. Flick J., Welakuh D. M., Ruggenthaler M., Appel H., Rubio A. (2019) Light-Matter Response in Nonrelativistic Quantum Electrodynamics, ACS Photonics, 6, 11, 2757–2778.

III) Making Polaritonic Coupled Cluster Machine Learnable

Among various approaches, the polaritonic quantum electrodynamics coupled cluster (QED-CC) method [1-2] offers a systematic way for describing the processes inside an optical cavity by treating electrons and photons quantum mechanically on the same footing. However, its applicability is hampered by the steep computational cost. The aim of this project is to develop a computationally efficient yet accurate alternative to the QED-CC method. This will be achieved by rewriting the QED-CC energy expressions in terms of electron density which in turn depends on the molecular grid [3]. As written in this form, we will utilize the correlation energy contribution at every grid point as a feature variable that will enter the machine learning model. The expected outcome of this project is to design and develop a predictive and computationally efficient machine learning model for accurate treatment of molecular polaritons. This project will make you familiar with high-performance computing systems, the python software language, and machine-learning concepts.

1. Haugland, T. S., Ronca, E., Kjønstad, E. F., Rubio, A., Koch, H. (2020). Coupled cluster theory for molecular polaritons: Changing ground and excited states. *Physical Review X*, *10*(4), 041043.
2. Pavošević, F., Flick, J. (2021). Polaritonic Unitary Coupled Cluster for Quantum Computations. *Journal of Physical Chemistry Letters 12*, 9100.
3. Margraf, J. T., Kunkel, C., Reuter, K. (2019). Towards density functional approximations from coupled cluster correlation energy densities. *The Journal of Chemical Physics*, *150*(24), 244116.

Quantum Monte Carlo

Contacts: Shiwei Zhang (szang@flatironinstitute.org) and Miguel Morales (mmorales@flatironinstitute.org)

The QMC group at Flatiron has broad interests. Our effort combines method/algorithm as well as software development with applications in diverse topics, for example: (a few recent publications are included for reference)

1. the study of strongly correlated electron models
   [arXiv:2202.11741 , arXiv:2112.02187]
2. ab initio computations in solids [arXiv:2204.12074 , arXiv:2011.08335]
3. quantum chemistry, transition metal and heavy element molecules
   [arXiv:2110.10201, arXiv:2001.07261]
4. Fermi gas and optical lattices with ultracold atoms
   [arXiv:2110.14493, arXiv:2110.06159]
5. boson and electron-phonon systems [arXiv:2008.03644, arXiv:2012.13473]
6. correlation effects in Moire materials

We have a number of projects suitable for the predoc program and encourage you to contact us if interested.