CCQ Summer 2022 Intern projects

CCQ expects to offer several research internships for the summer of 2022. Intern positions are intended for beginning graduate students and in exceptional circumstances advanced undergraduates. An application for an internship should include a statement of a preferred faculty supervisor and of preferred project.

Here is a list of potential projects for summer 2022 internships at CCQ. If you would like more information, please contact one of the scientists involved. Interns should feel free to propose projects of their own.

Strong light-matter coupling in molecular systems

Johannes Flick (jflick@flatironinstitute.org), Angel Rubio, Fabijan Pavosevic

So called 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 two possible research projects for summer research assistants. We also welcome your own ideas for research projects.

I) 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.

II) 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.


Symmetry of defect wavefunctions

Cyrus Dreyer (cdreyer-affiliate@flatironinstitute.org), Antoine Georges

Point defects are ubiquitous in all materials and can profoundly affect material properties. In addition, they can act as robust, isolated, manipulatable quantum systems for quantum computing, communication, and metrology. One of the key properties of a defect is the symmetry of the quantum states, which is determined by the chemical nature of the orbitals and the geometry of the crystal lattice. In this project, the intern will develop tools to automatically compute the symmetry of defect wavefunctions, so that they can be studied with a recently-developed quantum embedding methodology [1].

Adaptive Brillouin Zone Integration

Sophie Beck (sbeck@flatironinstitute.org), Jason Kaye, Olivier Parcollet

Brillouin zone integration is a standard operation in electronic structure calculations, required to compute system properties like the total energy and other physical observables. Such properties are often determined by highly localized features in momentum space. Numerical integration then requires a very fine momentum space grid, for example, in the presence of van Hove singularities, or when integrating over the Fermi surface, or energy-difference isosurfaces for calculations of optical conductivity. Using a roughly uniform spacing of integration nodes, as in most standard methods, is often insufficient to capture intricate details of electronic structure with a limited computational budget.

In scientific computing, adaptive integration methods are commonly used to resolve singular features of functions -- for example, corner and interface singularities in solutions of partial differential equations and boundary integral equations. However, their deployment for Brillouin zone integration has so far been limited, though a few methods have been proposed. Such an approach may provide a path towards the full resolution of localized features in momentum space, without a significant increase in computational cost. The proposed project would focus on exploring the viability of various methods for adaptive Brillouin zone integration, building robust software implementations of promising approaches for use by CCQ scientists and the broader physics community, and applying these implementations to challenging electronic structure calculations.


Development of data visualization WebApp FermiSee

Alex Hampel (ahampel@flatironinstitute.org), Sophie Beck

FermiSee (fermisee.flatironinstitute.org / github.com/TRIQS/FermiSee) is a recent web application to visualize and analyze spectral properties of the electronic structure of tight-binding models and realistic materials modeling. Target audience are scientists and students from theoretical or experimental backgrounds who wish to analyze electronic structure and correlation effects in a reproducible and interactive way. The visualized data of spectral functions can be linked directly to photoemission data measured in experiments. The project is an ideal opportunity to learn about fundamental properties of Green’s functions and the
connection between spectral functions calculated from tight-binding-like Hamiltonians and experiment. The app is written completely in python utilizing the in-house triqs library (triqs.github.io) for data processing, plotly and dash for visualization, and docker for web deployment. The project will focus on adding new features, such as fitting experimental spectral functions to extract insights from experimental data, or computing optical spectroscopy properties, enhancing the user experience of the App, and improving the performance.

Applicants should have an interest in data visualization, and app development. Prior knowledge of python including the scientific software stack, e.g. numpy and scipy is recommended. Basic understanding of electronic structure and the tight-binding method or Wannier90 (wannier.org) is helpful.

**Internship in Quantum Monte Carlo at CCQ**

Miguel Morales (mmorales@flatironinstitute.org), Bo Xiao, Paul (Yubo) Yang, Shiwei Zhang

Our work involves the development of algorithms and codes for quantum systems using stochastic approaches, and their application to tackle important problems in physics and chemistry. We have a number of projects appropriate for internships, focusing on methodology, software, or application. CCQ has a dynamic environment with many other members working on related problems. We welcome you to suggest/propose projects which can create synergy with us.

1. Properties of ultracold atoms in optical lattices. The goal is to perform accurate calculations to predict various correlations in these systems which are being realized with exquisite control in various laboratories. There are several possible projects here involving either finite-temperature or ground-state calculations. They employ auxiliary-field quantum Monte Carlo coupled self-consistently to gauge constraints using mean-field calculations. An internship project could be configured to focus on different aspects.

2. Correlated sampling in auxiliary-field quantum Monte Carlo. We have applied correlated sampling techniques to compute energy differences such as ionization potentials and bond dissociation energies in molecules. Current development has allowed us to study forces, stress, and phonon spectrum in solids. There are several projects involving the development and application of this technique in the study of properties of correlated systems including Hubbard models and Moire materials.