Master thesis: *Hybrid quantum-classical embedding simulations of materials*

Computational chemistry group, https://www.chem.uzh.ch/en/research/groups/hutter.html

The project

Quantum computing is set to revolutionize many fields of science, and quantum chemical and materials simulations have been identified as one of the most promising applications of this technology. However, current hardware is still limited in terms of size and complexity that can be dealt with, and new algorithms are needed to fully exploit the potential of this technology for materials simulations.

In this project, we plan to extend an active space embedding approach recently developed in our laboratory, which enables to perform electronic structure simulations of correlated materials in both the ground and the excited states.

Several developments to the current framework are possible, such as the implementation of state-specific and state-average orbital responses to account for environment relaxation effects, new short-range density functionals beyond the local density approximation, and the use of hardware-efficient quantum circuit ansatzes for obtaining the fragment Hamiltonian spectrum.

The developed methodology will be used to perform hybrid quantum-classical simulations of correlated materials, both pristine and with defects, focusing on excitonic and magnetic properties that are of interest for technological applications.

Your responsibilities / your tasks

Depending on the student's interests, the project can be either focused more on the development of the embedding framework, which requires good programming, analytical and mathematical skills, or, alternatively, more on the quantum simulations of correlated materials, whereby the student is expected to carry out the simulations and analyze the results.

We look for

We are looking for a motivated student in chemistry, physics, computational science, or any related discipline, ideally with previous experience in programming and electronic structure calculations, and with the willingness to learn about quantum computing.

We offer

The computational chemistry group headed by Prof. J. Hutter is a welcoming, friendly, and inclusive interdisciplinary research group, where the student will gain hands-on experience in electronic structure theory, materials modeling, and scientific computing. We offer a supportive environment, where the student can learn and progress, but also enjoy joint activities with the many international members of the group.

Place of work

University of Zurich, Department of Chemistry, Winterthurerstrasse 190, 8057 Zurich. The group is located in a brand-new building immersed in the nature of Irchel park, right at the heart of Zurich; Switzerland's largest city, renowned for its picturesque lakeside setting, financial and cultural significance, and high quality of life.

Application / contact details

For interest, please contact Dr. Stefano Battaglia (stefano.battaglia@chem.uzh.ch) with a short description of your scientific background and interests in the project.