Michele Pavanello Laboratory

Electronic structure theory and method development: In the Pavanello lab, the Scholar will be actively involved in the development of machine learning methods to describe electronic structures in molecules and materials. Initially, the Scholar will receive comprehensive training in basic Python programming, followed by an introduction to supervised machine learning techniques, including deep learning. This foundational training is anticipated to be completed within 2-3 weeks, ideally during the first summer period when the Scholar can dedicate her/himself to full-time work.

Following the initial training, the Scholar will undergo an additional 4 weeks of intensive instruction, focusing on fundamental concepts of quantum mechanics and delta-learning. During this phase, the Scholar will generate training data sets using advanced electronic structure methods, which will subsequently be utilized to train the machine learning model. By the end of the first summer period, the Scholar is expected to gather sufficient data to commence the drafting of a research manuscript.

The subsequent stages involve the thorough analysis and completion of the manuscript, along with the inclusion of necessary details. These tasks are distributed over the two semesters following the initial summer period and culminating with a journal publication. During the second summer, the Scholar will be ready to tackle a more complex project on linear and nonlinear optoelectronic properties of materials (the details will be defined at a later time and aligned with other current projects in the group). It is anticipated that during the second summer period the Scholar will generate data sufficient for another publication. This research experience can greatly benefit the Scholar's future endeavors, whether it be applying to graduate school or pursuing competitive positions in the industry.

During the summer period the Scholar will be working full-time on the assigned project. Throughout the academic year, a research commitment of 10 hours per week is expected. It is important to note that these are flexible guidelines and can be adjusted based on the Scholar's coursework and circumstances. Furthermore, due to the computational nature of the project, the Scholar has the flexibility to allocate some of their hours to remote work without compromising productivity or the overall quality of the experience. During the summer periods, I will hold weekly 1:1 meeting with the Scholar discussing the progress of the project. During the academic year the meetings will take place every other week. In both cases, the frequency can be increased as needed.

The Scholar will be fully integrated into my research group and, in addition to direct mentorship from me, will receive technical guidance from graduate students and postdocs in the lab. Scholars will contribute to lab meetings, presenting the results of their work and receiving feedback from lab members. We provide coaching on oral communication and presentations so that the Scholar feels comfortable conveying their findings and we expect the Scholar to prepare a poster for conferences as well. As Mentor, I will ensure that the Scholar is well-trained in the search for relevant literature and to become familiar with the scientific writing in this field to prepare the Scholar to write manuscripts for submission to leading journals. Fellow group members and I will advise the Scholar on the factors to consider when the selecting the best suited graduate program, how to compose the CV, and the personal statement letter.