Etienne Palos

EXPAND Mentor

Understanding the complexity of chemical systems: many-body physics meets computational chemistry

Dr. Francesco Paesani / Paesani Lab (Winter, 2021-22)

What you will do

Have you ever wondered how the physical properties of a single water molecule differ from those of "bulk" liquid water? The difference lies in the *complexity* of the systems. Specifically, in the case of bulk water, there are N water molecules (where N is a very large number) that are simultaneously interacting with each other, exchanging energy and momentum, and moving around - rearranging the *network* of hydrogen bonds that defines the structure of water as we see it. Such interactions are known as many-body (MB) interactions. In reality, all physical and chemical systems are composed of complex networks of interacting constituents. While it seems clear that understanding these MB interactions can further, and complete, our understanding of chemistry, traditional theoretical models fail at describing the properties of chemical systems (such as water) from the gas (small N) to the condensed phase (very large N). **In this project, you will tackle the complexity of chemical systems from the gas to the condensed phase, with computer simulations that combine many-body physics with machine learning.** Throughout this experience, you will learn to execute quantum mechanical (electronic structure) calculations as well as dynamical simulations (MB molecular dynamics) of your chemical system. Moreover, you will actively learn and combine techniques from mathematics, computer programming, as well as physics and chemistry, that will provide you with a quantitative skill set that is translatable to any field of knowledge or career path.

Skills you will acquire

- Understanding the role of high-performance computing in scientific research

- Familiarity with modern quantum and statistical physics

- Mastery of data analysis with Python libraries

- Fluency in working in a computational environment using Linux

- Capability to think critically about complexity; connecting individual and collective properties