Atomic Scale Simulations with Machine Learning Techniques for Post-Lithium Battery Materials

The aim of the project is the characterization of the interfaces between electrode and electrolyte in sodium batteries, an emerging alternative technology to lithium-ion batteries. We will use numerical simulations with molecular dynamics techniques to understand the composition, structure, and role of the solid-electrolyte interphase (SEI) that forms at the solid/liquid interface in these devices. Specifically, we will develop machine-learning-based interatomic potentials trained on data obtained from electronic structure methods (density functional theory, DFT) to perform large-scale simulations with DFT-level accuracy and computational efficiency comparable to classical force fields. In collaboration with our experimental partners (mostly based in Japan), we expect to gain a better understanding of the role of the SEI in electrode stability and sodium ion transport kinetics across the interface.

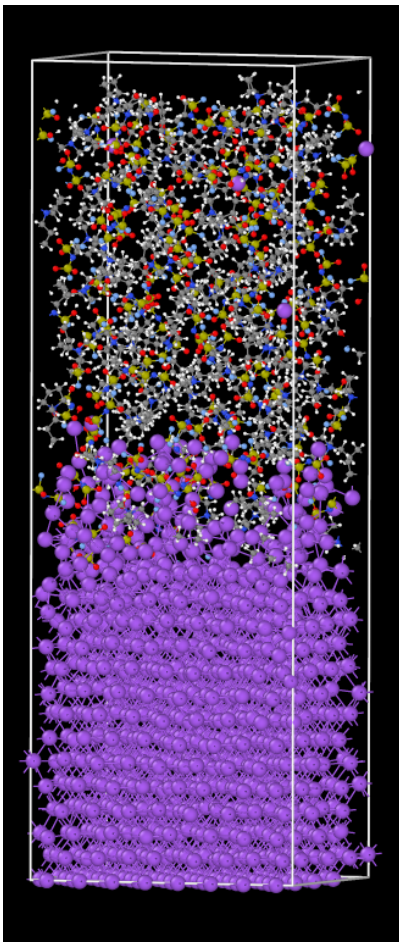

Figure 1: Model of the interface between the Na-metal electrode and an ionic liquid electrolyte

Sodium-ion batteries are an emerging technology offering significant advantages over established lithium-based batteries in terms of stability and the availability of raw materials. Working closely with our experimental partners, we aim to gain better insight into the operation of hard-carbon-based anodes, currently the most promising material for this crucial battery component. This work is part of several ongoing initiatives led by the project's Principal Investigator on this topic. Notably, in 2025, a cooperative project between Italy and Japan on sodium-ion batteries was launched. Japanese collaborators include experimental groups, especially that of Prof. Komaba (Tokyo University of Science), a pioneer in sodium batteries, and theory partners like Prof. Yoshitaka Tateyama (Institute of Science Tokyo), an expert in numerical simulations of electrochemical processes. The PI is also leading a project in partnership with ENI S.p.A. on sodium-metal batteries, in collaboration with various Italian academic partners.