

Computational multiscale approach to finding improved materials and architectures for the next battery generation

Understanding a battery's performance requires having an in-depth knowledge of a plethora of phenomena that occur in a wide range of length and time scales. The length scales span from the atomistic level for describing electrochemical reactions and ion transport to the device level for developing battery management systems (see Fig. 1). Similarly, the time scale spans from picoseconds for reactions and transport to years when describing the aging and shelf life. Albeit accurate and widely used modeling methods at different length and time scales exist, they are almost always used independently of other scales.

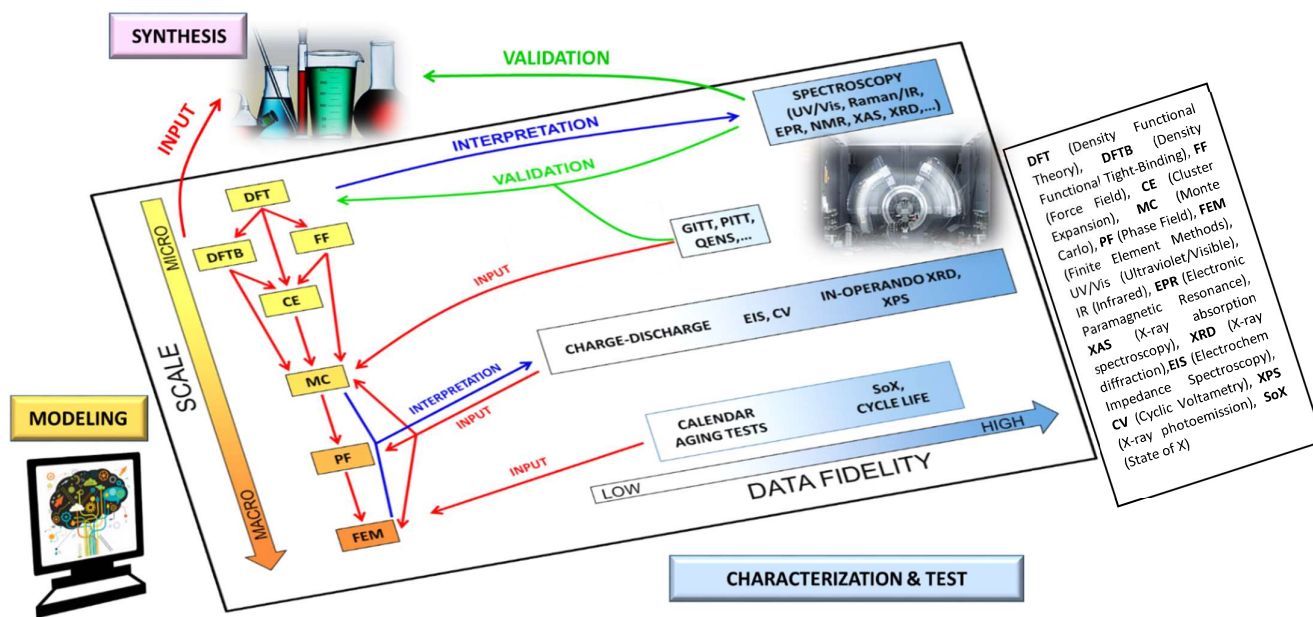


Figure 1. The intricate interconnection between Modeling, Synthesis, and Characterization and Testing experiments in Battery research.

The ultimate challenge in battery modeling lies in the lack of a reliable multiscale modeling method that accounts for processes occurring in different scales. Ideally, the parameters for mesoscopic and macroscopic simulations would derive from a set of relevant experiments combined with the output of microscopic scale calculations (see Fig. 1). As I will describe during the lecture, machine learning algorithms can help build robust multiscale modeling frameworks by tackling three crucial aspects: i) Development of more accurate microscopic models that account for real operando conditions. ii) The ability to act as a "glue" that helps to connect different simulation scales. iii) Enhancement of an integrated closed-loop between theory and experiments, i.e., to optimize the inclusion of experimental data in simulations, and concomitantly, to forecast complex experimental outcomes (e.g., battery aging or materials synthesizability) from theoretical models.