Ph.D. School in Chemical Sciences
Cycle XXXVIII

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Research project title: Digital design of functional materials for energy conversion and storage devices

Key words Computational chemistry; Multiscale simulation; Machine learning; Electrode-electrolyte interface; Electrochemical device

Research project abstract The working principles in energy storage and conversion devices usually involve complex charge and mass transport mechanisms occurring at electrode-electrolyte interface that are strictly dependent on several aspects. Computational modeling plays a key role in this field as it can provide the suitable tools to untangle these factors, to provide new insights on the structureproperty-function relationships towards the design of new and more efficient materials. The goal of this project consists in developing innovative theoretical methods able to describe any electrode-electrolyte interface with reliable predictions at affordable costs. The main interactions between promising electrode and electrolyte materials (Na metal, layered transition metal oxides, polymer and polymer/nanoparticles hybrid membranes) will be explored and the transport mechanisms at the related interfaces will be addressed by using metadynamics simulations combined to artificial intelligence tools.