In spite of its technological relevance in the energy conversion and storage, our knowledge about the microscopic structure of electrochemical electrode-electrolyte interfaces is still rather limited. This is particularly true for electrochemical interfaces in batteries which typically exhibit an ill-defined structure [1].

In this contribution, we will present our attempts to contribute to, to a deeper understanding based on electronic structure calculations by systematically increasing the complexity of the considered systems.

We will discuss the surface structures of both anode and cathode materials. Dendrite growth in Lithium-ion batteries represents a severe problem as it can lead to short-circuits in the battery, rapid overheating and sometimes even fire. Magnesium, on the other hand, does apparently not show a tendency towards dendrite growth. We have focused on basic metal properties in order to understand these difference between Li and Mg [2].

Furthermore, we address the stability of oxidic cathode materials. They can exhibit polar surfaces which can be sometimes surprisingly stable due to a polarity compensation mechanism [3]. Finally, the challenges in modeling electrode/electrolyte interfaces [1] will be discussed, in particular as far as liquid electrolytes are concerned.

References