DFT *ab initio* Molecular Dynamics Simulations of Lithium-metal Rechargeable Batteries

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For environmental and economic reasons, it is very important to develop efficient, robust, light, and safe batteries for vehicular transport. One possible alternative is the use of Li-metal as the anode, which implies a theoretical gravimetric energy density 10 times that of graphite, which is the standard anode of widely used lithium-ion batteries (LIBs). In this presentation, I will show our ongoing efforts to determine the proper electrolyte components capable of passivating the highly reactive metal anode by forming a solid electrolyte interphase (SEI) during the first few operating cycles of a lithium metal battery (LMB). The interphase formed is expected to protect both the anode and the electrolyte, be a good insulator for electrons but a good conductor for lithium ions. Furthermore, these characteristics must be maintained under compression and stress of the metal due to lithium deposition and extraction during the charge and discharge periods, respectively. Thus, to understand the creation, evolution, and characterization of the SEI, we use ab initio procedures to assess electronic structure and dynamics under reactive environments. Ab initio studies complement very well the few existing experimental techniques. To complicate matters in the decision to use molecular or extended methods, SEI is primarily an amorphous, non-stoichiometric material, created primarily during charging, hence under external electrical potential, and is the key to determining the performance of a battery. Therefore, to know and understand SEI properties, we have studied the behavior of typical electrolytes used in LIB and new ones developed for LMB, such as high concentration electrolytes and localized high concentration electrolytes, as well as ionic liquids and solid state. electrolytes, giving us the reaction pathways of electrolytes, the evolution of SEI composition, and the effects of some electrolyte additives.