Molecular Modeling of Electrochemical Interfaces for Energy Conversion

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The absolute majority of electrochemical processes are defined as taking place at the electrochemical interfaces comprising an electronic or a mixed conductor (electrode) and ionic one (electrolyte). These processes also form the functional basis of electrochemical energy conversion devices: batteries, fuel cells, supercapacitors etc. that are recently receiving increasing attention due to the developments in renewable energy.

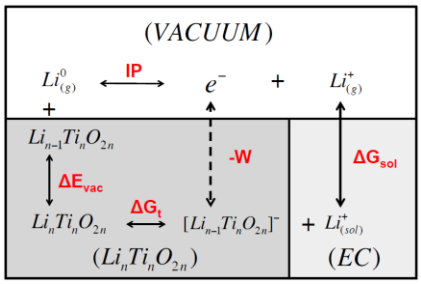

Fig. 1 Thermodynamic Born-Haber cycle for the electrochemical delithiation of $Li_xTi_2O_4$ spinel at the interface with ethylene carbonate based electrolyte.

Modern molecular modeling techniques such as density functional theory and molecular dynamics provide unprecedented detail and insight into these processes with an atomic spatial and temporary resolution unattainable to any experimental method.

We will present our recent results in modelling various Li/Na-ion battery interfaces using different methodologies and scales as well as what are the critical issues and limitations of these approaches. In addition, we will discuss how these results help to elucidate the fundamental questions regarding the function and problems of electrochemical energy conversion systems.

REFERNCES

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