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MATERIALS GENOME INITIATIVE SEMINAR SERIES

Towards predictive *ab initio* simulation of surfaces and interfaces

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ABSTRACT The Interface between electrode and electrolyte is one of the most important factors, which determines the efficiency of the energy conversion and storage devices, such as fuel cell, solar cell, and battery. Understanding the interface structure and electronic properties is of fundamental importance for the development of new and efficient devises. Periodic density functional theory (DFT) within the local density approximation (LDA) and generalized gradient approximation (GGA) has been routinely used to gain insight into the electrode-electrolyte interface. Yet, the accurate and efficient methods need to be developed to describe the electrochemical interfaces, i.e., electrified interface between electrode and electrolyte.

In this talk, I introduce a method called the effective screening medium (ESM) method[1,2], which enable one to simulate the electrified interface efficiently using a slab geometry. I also discuss recent progress of the van der Waals density functional (vdW-DF)[3-5]. The functional can capture the van der Waals forces, which are essential in the electrode-electrolyte and elctrolyte-electrolyte interfaces.

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