Influence of polarization and chemical environment on the stability of Pt/PTO/Pt capacitors

Miguel Angel Méndez Polanco, Ilya Grinberg, and Andrew M. Rappe

The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania.

Philadelphia, Pennsylvania 19104-6323, USA.

The ferroelectric polarization of perovskite oxides can be utilized in the production of non-volatile memory applications. In order to develop high density storage devices, it is crucial to study and understand the existence of a critical size for the stabilization of ferroelectricity in ultra-thin capacitors and the interactions occurring at the metal/oxide interface play an important role on determining their properties and stability.

We have used Density Functional Theory to investigate the structure and stability of $Pt/PbTiO_3/Pt$ capacitors focusing on the effect of polarization on the adsorption preference of Pt when deposited on the (001) ferroelectric surfaces of PbO-terminated $PbTiO_3$ thin films. We found that the preferential site deposition depends on the polarization of the oxide surface and, on the thin-film size regime, this effect gives rise to the appearance of asymmetric capacitors in otherwise chemically symmetric devices. Analysis of the energetics as thicker metal electrodes are grown on the capacitors, and the exploration of its connection to their local geometrical structure, manifest the strong relationship between the ferroelectric stability and the chemical environment at the interfaces.