DF 3: Dielectric surfaces and interfaces

Time: Monday 10:30–10:50 Location: H11

DF 3.1 Mon 10:30 H11

First principles simulation of a moving longitudinal domain wall in $PbTiO_3$ — •Kourosh Rahmanizadeh, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In ferroelectrics, the formation of domain walls can compensate the surface charge, release elastic strain and lower the free energy of the crystal. However, 180° head-to-head domain walls are energetically costly due to electrostatic repulsion of charges at the interface. It is possible to reduce the electrostatic energy at the longitudinal domain wall by including electron donors / acceptors.

We carried out density functional theory calculations based on the full-potential linearized augmented planewave (FLAPW) method as implemented in the `FLEUR` code (www.flapw.de) for simulating domain walls in $PbTiO_3$. To stabilize these walls, we introduce effective Ti and O vacancies for accepting and donating electrons.

We modeled the growth of domains with different configurations of the vacancies. For each configuration, the structures were optimized. We also investigated the pinning strength of domain walls in $PbTiO_3$. To this end, we applied external electric fields ranging up to 9×10^7 V/cm to the simulated structures, monitoring the evolution of the total energy.

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