

# Zigzag charged domain walls in ferroelectric BiFeO<sub>3</sub>

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Domain walls in ferroelectrics are usually electrically neutral because charged walls lead to very strong depolarizing fields, which would effectively suppress such a domain arrangement. The experimental observations of charged walls can be explained by the presence of different kinds of defects, which can compensate for the bound charge originating from the polarization variation at the wall. Previous theoretical studies of charged walls usually assumed that the compensation charges are very localized.

In this talk, I will address a charged 180° domain wall in ferroelectric PbTiO<sub>3</sub>, which is compensated by static charges distributed randomly in a relatively broad layer. We use atomistic simulations to obtain details of the domain-wall microstructure. For larger compensation-layer thicknesses, we utilize phase-field simulations within the framework of the Ginzburg-Landau-Devonshire model (As it is our main tool, I will introduce the phase-field method in a little bit more detail). The atomistic and the phenomenological approaches predict a zig-zag domain wall located within the compensation layer. I will discuss the internal structure of the domain wall, and how it depends on the thickness of the compensation region.

In the final part of my talk, I will present the theoretical predictions obtained for a similar domain wall in rhombohedral BiFeO<sub>3</sub>, and compare these with experimental results recently published by the Microscopy Group at the University of Warwick.