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Lattice screening of the polar catastrophe in $KNbO_3/BaTiO_3$ interfaces PABLO GARCIA-FERNANDEZ, PABLO AGUADO-PUENTE, JAVIER JUNQUERA, CITIMAC, Universidad de Cantabria, Avda. de los Castros s/n, E-39005 Santander, Spain — The discovery of a bidimensional electron gas (2DEG) in the interface between two insulating lattices like $LaAlO_3$ and $SrTiO_3$ has triggered much interest around bidimensional conductivity in these heterostructures. In this work we study polar interfaces between $KNbO_3$ (KNO) and $BaTiO_3$ (BTO), equivalent from the layer by layer charge point of view to the LAO/STO. In particular we focus on: (a) the possibility of formation of a 2DEG, (b) its interaction with the ferroelectric distortions of these materials, and (c) the effect of external electric fields. For this, we have performed Density Functional Theory calculations for a KNO(m)/BTO($2m$)/KNO(m) slab (m= width in unit cells) with different kinds of interfaces (n or p). We find that a 2DEG is formed only in the unrelaxed configuration, where there is no rumpling between the atoms of a given layer. However, when geometry is relaxed, $KNbO_3$ polarizes and the 2DEG is effectively screened. This effect is robust even under application of electric fields of moderate size. Finally, we find that an easily-rotated [110] in-plane polarization, driven by electrostatic effects, appears in the vicinity of the KO/TiO_2-type interface even thought the system is under in-plane compressive strain.

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