Effect of surface steps on the ferroelectricity of $PbTiO_3$: A first-principles study

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Abstract

In this study, *Ab initio* (first-principles) density functional theory (DFT) calculations are performed within the local density approximations (LDA) to investigate the ferroelectricity at $PbTiO_3$ surface steps consisting of (001) and (100) surfaces with a spontaneous polarization along[100]. For both the PbO- and TiO_2-terminated surface steps, the [100] polarization is suppressed and the [001] polarization appears at their upper terraces, which results in a rotation of polarizations at the surface steps. The polarization rotation is induced by the local variation of the covalent Pb–O bond due to the charge redistribution at the surface steps. Furthermore, we investigate the interaction of the surface steps. Although surface steps with the same polarization configuration exhibit little interaction, steps of different types interact with each other strongly, suppressing the ferroelectricity, especially on the upper terrace.

Keywords: Ferroelectricity, surface step, $PbTiO_3$, First-principles study