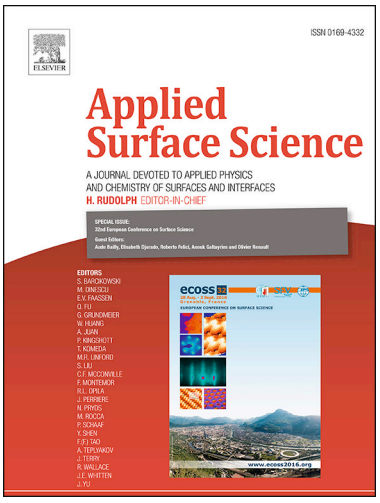

Full Length Article

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Magnetism and multiferroic properties at $MnTiO_3$ surfaces: A DFT study

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Keywords: $MnTiO_3$, magnetism, multiferroic properties, morphology, Wulff's construction, surface energy, spin density.

ABSTRACT: The present study illustrates how density functional theory calculations can rationalize the surface structure and magnetism for the low-index (110), (101), (100), (001), (111), and (012) surfaces of $MnTiO_3$. A simple procedure, without surface reconstructions or chemical adsorptions in which the stability, magnetism and the morphological transformations is presented in detail to clarify the control of their multiferroic nature. The surface stability was found to be controlled by the octahedral [MnO_6] and [TiO_6] clusters formed by the Mn^{2+} and Ti^{4+} cations - i.e., their local coordination at the surfaces, respectively- with nonpolar (110) being the most stable. Enhanced superficial magnetism was found for (012), (001), and (111) surfaces in