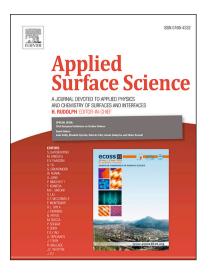
#### Accepted Manuscript

#### Full Length Article

Magnetism and multiferroic properties at MnTiO<sub>3</sub> surfaces: A DFT study

Renan A.P. Ribeiro, Juan Andrés, Elson Longo, Sergio R. de Lázaro

PII:	\$0169-4332(18)31360-6
DOI:	https://doi.org/10.1016/j.apsusc.2018.05.067
Reference:	APSUSC 39343
To appear in:	Applied Surface Science
Received Date:	19 April 2018
Accepted Date:	9 May 2018



Please cite this article as: R.A.P. Ribeiro, J. Andrés, E. Longo, S.R. de Lázaro, Magnetism and multiferroic properties at MnTiO<sub>3</sub> surfaces: A DFT study, *Applied Surface Science* (2018), doi: https://doi.org/10.1016/j.apsusc. 2018.05.067

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

### **ACCEPTED MANUSCRIPT**

# Magnetism and multiferroic properties at MnTiO<sub>3</sub> surfaces: A DFT study

Renan A. P. Renan A. P. Ribeiro<sup>a</sup>, Juan Andrés<sup>b,\*</sup>, Elson Longo<sup>c</sup> and Sergio R. de Lázaro<sup>a</sup>

<sup>a</sup>Department of Chemistry, State University of Ponta Grossa, Av. General Carlos Cavalcanti, 4748, 84030-900, Ponta Grossa, PR, Brazil

<sup>b</sup>Department of Analytical and Physical Chemistry, University Jaume I (UJI), Castelló 12071, Spain.

<sup>°</sup>CDMF-UFSCar, Universidade Federal de São Carlos, PO Box 676, 13565–905 São Carlos, SP, Brazil.

Keywords: MnTiO<sub>3</sub>, 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<sub>3</sub>. 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<sub>6</sub>] and [TiO<sub>6</sub>] clusters formed by the Mn<sup>2+</sup> and Ti<sup>4+</sup> 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

Download English Version:

## https://daneshyari.com/en/article/7833507

Download Persian Version:

https://daneshyari.com/article/7833507

Daneshyari.com