

Accepted Manuscript

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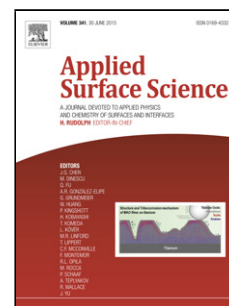
PII: S0169-4332(17)32789-7
DOI: <http://dx.doi.org/10.1016/j.apsusc.2017.09.141>
Reference: APSUSC 37220

To appear in: *APSUSC*

Received date: 10-3-2017
Revised date: 1-9-2017
Accepted date: 17-9-2017

Please cite this article as: Estefania German, Ricardo Faccio, Alvaro W. Mombrú, Comparison of standard DFT and Hubbard-DFT methods in structural and electronic properties of TiO₂ polymorphs and H-titanate ultrathin sheets for DSSC application, *Applied Surface Science* <http://dx.doi.org/10.1016/j.apsusc.2017.09.141>

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Comparison of standard DFT and Hubbard-DFT methods in structural and electronic properties of TiO₂ polymorphs and H-titanate ultrathin sheets for DSSC application

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Highlights

- DFT and DFT+U comparison in TiO₂ polymorphs and Hydrogen titanate surfaces
- Implementing Hubbard term improves the electronic properties calculation
- Hubbard term addition does not affect significantly structural and energetic properties
- Our results helps to understand the behavior and applications of these surfaces in DSSC

Abstract

The structural and electronic properties of several TiO₂ polymorphs and hydrogen titanate surfaces are modeled and studied by density functional theory (DFT). By implementing the Hubbard parameter "U" in our calculations more realistic results of electronic properties are obtained, paying with a small deviation in geometric optimization. Lattice parameters difference is found to be less than 6.2%, as well as some changes in surface energy are found, but the reactivity tendency of

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