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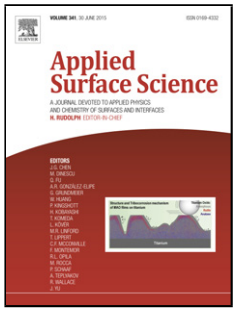

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Comparison of standard DFT and Hubbard-DFT methods in structural and electronic properties of TiO_2 polymorphs and H-titanate ultrathin sheets for DSSC application

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Highlights

- DFT and DFT+U comparison in TiO_2 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 TiO_2 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