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Analysis of the interaction of water with TiO_2 nanotubes

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Abstract: TiO_2 is a multifunctional semiconductor that presents a wide variety of applications in different fields, such as: ceramic, cosmetic, catalyses, etc [1, 2]. At atmospheric pressure, TiO_2 presents three stable polymorphs: rutile, which is thermodynamically favored, anatase and brokita. These polymorphs show different degrees of chemical reactivity and studies have shown that the TiO_2 anatase is more reactive when used for catalysis and photocatalysis studies. The TiO_2 anatase, focus of this study, presents a tetragonal structure formed by clusters [TiO_6]. In this work a study of the TiO_2 nanotubes and the interactions with the water molecule were carried out. The CRYSTAL14 program associated to DFT and to the B3LYP hybrid functional was used. The theoretical results of the nanotubes were correlated with experimental data of the group and those found in the literature.

Key-words: TiO_2 anatase, nanotubes, DFT.
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