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A Density Functional Theory Study of Electronic Structure of TiO_2 Rutile (110) Surfaces with Catechol Adsorbate

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Titanium dioxide (TiO_2) is used as semiconductor in the dye sensitized solar cell (DSSC), amongst many other applications. Thus coupled with a suitable sensitizer such as catechol, the study of surface electronic structure of TiO_2 will improve light harvesting and electron transfer processes in DSSC. The distribution of states in clean and catechol terminated four and five layer TiO_2 (110) rutile surfaces were investigated. All calculations in this work were done by quantum espresso code which uses plane waves and pseudopotentials. The slabs were modelled by four and five layers with vacuum width of 20 Å. The results showed that the (110) stoichiometric TiO_2 four layer surface had band gap of 2.1 eV, a value less than band gap value of 2.2 eV of similar catechol bound TiO_2 surface. There was an increase in the band gap value of 0.32 eV for the catechol bound TiO_2 (110) rutile five layer surface compared to that of clean stoichiometric TiO_2 (110) surface. The HOMO in four and five layered TiO_2 (110) surfaces was found to lie above the valence band edge. The LUMO in both surfaces was located in the conduction band, and hence the band gap of the molecule was in the range of 4.0 eV. These findings have showed that the energy level alignment of catechol coupled to TiO_2 is a suitable model to study electron transfer processes that occur in dye sensitized solar cell.