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Fundamental properties of TiO_2 nanostructures: the effects of the size confinement and the surface coverage GIOVANNI CANTELE, CNR-INFM-Coherentia, Universita' di Napoli Federico II , Naples, Italy, AMILCARE IACOMINO, Universita' di Roma Tre and CNISM, U. di R. Napoli, Naples, Italy, FABIO TRANI, DOMENICO NINNO, Universita' di Napoli Federico II, Naples, Italy, IVAN MARRI, STEFANO OSSICINI, CNR-INFM-S^3, Universita' di Modena e Reggio Emilia, Modena, Italy — The titanium dioxide (TiO_2) complexes are widely investigated for their multipurpose capabilities. We discuss here a characterization of anatase TiO_2 0D clusters (NCs) and 1D nanowires (NWs) in the framework of ab initio DFT calculations. Based on both theoretical and experimental evidences, we defined an anatase TiO_2 NC by modifying a perfect bipyramidal morphology and then used this NC as a chain repetition unit in the anatase NW. We studied the size confinement and analyzed the effect of surface coverage by functionalization with simple water-derived adsorbates. We found that the structural reconstruction fit the available experimental data, that the band gap shift depends on the crystallinity and that the hydration is important in stabilizing the nanostructures.

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