Theoretical Study of the Electronic Structure and Stability of Titanium Dioxide Clusters $(TiO_2)n$ with n=18, 28, and 38.

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TiO2 is an active semiconductor used in photocatalysis, solar cells devices and energy storage applications. For this reason, recent efforts are aimed to design and modify the properties of this semiconductor. In the present work we calculate theoretically the lowest energy structures of TiO2, and The Density of States (DOS) using Molecular Dynamics and DFT respectively. Such geometries were compared with those reported experimentally, and their atomic structures were constructed with planes (1 0 1) of anatase symmetry. The nanoparticles considered were (TiO2)n with n=18, 28, and 38. The aim of this work is to correlate the size dependence of TiO2 nanoparticles with temperature effects on anatasa simmetry. A quenching process was used in order to reproduce the temperature conditions found at experiment. Also, The RDFs (Radial Distribution Function) of these materials were obtained. The DOS were determined using Density Functional Theory (DFT) calculations, it was implemented with FHI-AIMS software package [1,2], and Molecular Dynamics using DL-POLY[3] and REAXFF software packages [4,5]. The DFT calculations were performed using a plane-wave basis set, and the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof for the exchange-correlation energy [6]. The core electrons were described with Projector Augmented Wave (PWA) method. Moreover, relativistic scalars effects (ZORA)[7] and Van Der Waals interactions were considered using Tkatchenko-Scheffler methodology[8].

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