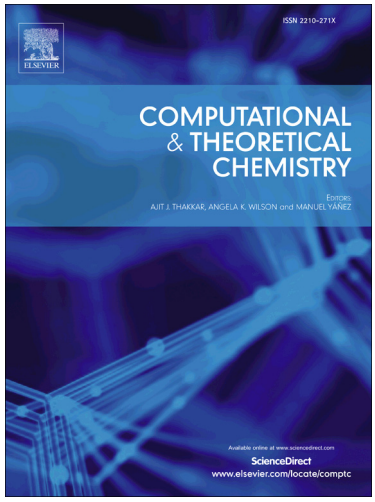

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Theoretical investigation of electron structure and surface morphology of titanium dioxide anatase nano-particles.

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Abstract

Titanium dioxide is a widely used material. It is white pigment and a very effective UV filter, nano-particles of titanium dioxide show effective photocatalytic properties. Also, it is used in the manufacturing of dye-sensitized solar cells. Recent experimental studies show that the properties (e.g. photocatalytic performance, adsorption, reflectance, adhesion, carrier transportation properties, nano-toxcity, etc.) of the titanium dioxide nano-particles are dependent on their shape, sizes and surface morphology. Therefore, both experimental and computational study of TiO2 nano-clusters and the development of both experimental and computational techniques for the study are the actual goals. Thus, in the current work, a theoretical study of anatase nano-particles, their shape, electron characteristics, surface morphology, the influence on adsorption has been performed. A new methodology based on AlteQ approach for the accurate estimation of the electron density, surface, volume characteristics in a reasonable time for theoretical study of nineteen anatase nano-clusters of different forms (cub, ellipsoid, sphere, cuboid) and sizes from $Ti_{25}O_{50}$ to $Ti_{650}O_{1300}$ has been applied. The comparison of the AlteQ and the first principles methods has been performed and the applicability of the AlteQ approach has been confirmed. The computations have been performed at http://www.chemosophia.com/ using "Electron properties calculation: Integration over atomic basins" software. The study showed that the ratio of the summary atomic external surface area of oxygens varies in the wide range 0.42÷0.65 dependently on the shape and the surface morphology of a nano-cluster. The maximal values (0.52÷0.65) are typical of elongated nano-clusters with deep and long furrows observed on the faces parallel to *c* axis while the least values (0.42 ÷ 0.43) are observed in the cases of spherical nano-clusters with smoother surface. Thus, elongated TiO_2 nano-clusters with deep