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Characterization of Anatase Nanoparticles Using Tight Bonding DFT Simulation HONG WANG, NING MA, HAO WANG, JAMES P. LEWIS, Department of Physics, West Virginia University, CONDENSED MATTER COMPUTAIONAL GROUP TEAM — The structure and electronic properties of anatase nanoparticles with size ranging from 1.5nm to 2.4 nm have been presented in this paper under ab initio Density Functional Theory computational method. Based on the relaxed structures obtained in our calculation, we propose that the portion of surface in the whole structure effects the geometric configuration of anatase nanoparticles. However, as long as the nanoparticles grow bigger, the affection decreases obviously. The analysis of the frontier orbitals of the nanoparticles in our work make us believe that the frontier orbitals (so called HOMOs) are mostly localized on some corner positions of the whole structure. These corner positions are constisted of 4-coordinated Ti atom lack of bridge oxygen atoms. When we adsorb water molecule on different positions on the facets of the smallest particle $(TiO_2)_{48}$, it turns out the corner position where the frontier orbitals are mostly localized are most energetic favorable adsorption position for water molecule. These special corner positions will likely act as high attractive spots for the external molecules existing in the nanoparticles' environment.

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