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Where the reactive sites are in anatase nanoparticles? – Theoretical Investigation on (001) and (101) surfaces in anatase nanoparticles HONG WANG, JAMES LEWIS, West Virginia University — Recently, with the development of nanotechnology, the devices' size shrinks to nano-scale size where the surface properties play a role. Thus, it is required scientists to provide fundamental level understanding of anatase surfaces in nano-size anatase materials to improve its applications. In this work, applying DFT ab initio method, we investigate the fundamental properties of anatase (001) and (101) surfaces in anatase nanoparticles. By adopting different portions of (001) and (101) surfaces along with the size of nanoparticles, we analyze the geometric properties and energetic stabilities of nanoparticles. The electronic properties of these nanoparticles are also calculated in this work. The frontier orbitals located mostly in the (001) surfaces indicate these sizes are possibly reactive sizes in the external molecule adsorption reactions. To verify their activity, we add water molecules in different sits and different concentration on these nanoparticles. The results show that the sites where the frontier orbitals are localizing are very reactive for water adsorption.

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