# Photo- and electrochemistry of charge trapping sites on anatase-type $TiO_2$ nanoparticles - a theoretical perspective

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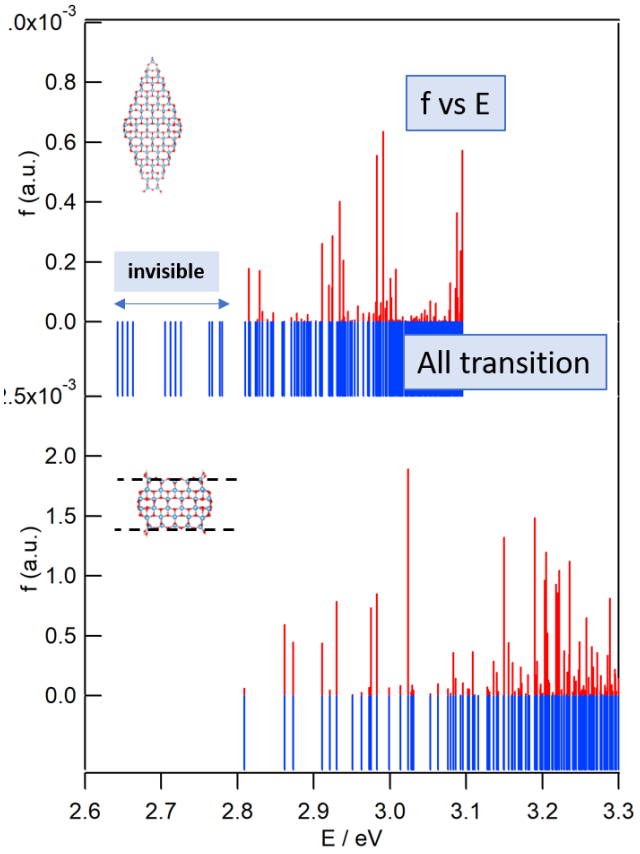
Oxide nanoparticles, like $TiO_2$ nanoparticles are often applied in electrodes and photocatalytic systems. The morphology and shape of these nanoparticles can be easily tuned with experimental conditions, which raise the question how much the electro- and photochemical properties are affected by the nanoparticle geometry.

We studied the electronic states around the bandgap in anatase-type $TiO_2$ nanoparticles of different shapes with (101) and (001) facets using Density Functional based Tight Binding (DFTB) method as implemented in DFTB+ (ver. 19.1, SCC-DFTB and TD-DFTB, Cassida method). Previous calculation has already shown that most orbitals of the valence and conduction bands forms delocalized band-like orbitals, however there are a significant number localized states, especially at the lower at edge of conduction band, too. These trapping sites may play important role in electrochemistry when placed on the surface of the nanoparticle. Due to the relatively low number of atoms on the surface, and the significantly higher activity of low energy catalytic sites, charge trapping can control the electrochemical properties.




Photochemical properties however depend on optical transitions between electronic states with given symmetry, and mostly dominated by delocalized states of atoms in the bulk. In this talk we analyze the optical spectra (see Figure) on the nanoparticles and compare it to the electrochemically important surface trapping