Orientation effects in electronic properties of TiO$_2$ nanowires and nanotubes in the rutile and anatase phases.

By

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Host: Asst. Prof. Cesare Soci

Abstract
In this talk we report our results of *ab initio* calculations that show the influence of morphology on electronic properties of TiO$_2$ nanowires and nanotubes both in the rutile and anatase phases. In the case of rutile TiO$_2$ nanowires a nice possibility of band-gap engineering by introducing different facets is revealed. Appearance of flat bands in the gap region for some nanowire orientations is also discussed. Anatase TiO$_2$ nanowires and nanotubes with the same orientation are found to display similar dispersion of bands near the gap region. Finally, we clarify the role of quantum confinement effects in the band-gap variation of TiO$_2$ nanowires and nanotubes.

Short Biography