Nowadays TiO$_2$ nanoparticles are widely employed in photocatalysis and in dye sensitized solar cells. In these applications the relevant phenomena are occurring at the surface of the nanoparticles, therefore the investigation of the relations between particles morphology and surface properties is crucial to understand their reactivity and to improve their performance. Spectroscopic methods are very effective in unravelling structure and reactivity of oxide surface sites. In particular, IR spectroscopy of adsorbed carbon monoxide, used as molecular probe, allows obtaining information at molecular level on the different exposed surfaces. This talk will show that the spectroscopic results combined with first-principles calculations and electron microscopy provide a powerful tool to correlate the spectral features with surface properties and particles morphology [1, 2].

The information obtained with this approach represents the initial point for the investigation of the reactivity of the different nanoparticles surfaces. As an example, the possibility to growth in situ...
graphene-like layers by self-assembly of molecular precursors (e.g. C$_2$H$_2$) on the TiO$_2$ surface will be presented [3].

The last part of the talk will discuss the use of spectroscopic techniques to study the processes occurring at the TiO$_2$ surface during photocatalytic reactions. Indeed, in situ IR spectroscopy allows monitoring the evolution of the reaction intermediates and products at the photocatalyst surface in controlled atmosphere, after sending well-defined doses of reactants. This approach helps to better understand the reaction mechanism and to determine the degradation kinetics in different surface conditions [4].