

Doping is one of the most common strategies for improving the photocatalytic and solar energy conversion properties of TiO<sub>2</sub>, hence an accurate theoretical description of the electronic and optical properties of doped TiO<sub>2</sub> is of both scientific and practical interest. In this talk I will present the electronic structure, optical absorption spectra and excitonic properties of H- and Nb- doped TiO<sub>2</sub> calculated by ab initio calculations based on density functional theory, GW approximation and Bethe-Salpeter equation. Our results show defect energy levels, lying in the energy gap, which are also responsible for the appearance of low energy absorption peaks that enhance the solar spectrum absorption of TiO<sub>2</sub>. The spatial distribution of the excitonic wavefunctions associated with these low-energy excitations are very different for the two dopants, suggesting different mobility of photoexcited electrons in doped TiO<sub>2</sub>.