

## Surface defects and doping in TiO<sub>2</sub>

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Titanium dioxide, TiO<sub>2</sub>, is a widely used, yet quite inefficient photocatalyst. Among the important drawbacks, its band gap is rather large for efficient use of sunlight, and control of trapping and recombination sites for photo-excited carriers is very limited.

In this talk I will present results of theoretical studies aimed at obtaining insights into issues relevant to TiO<sub>2</sub>-based photocatalysis. In particular, I will discuss the geometric and electronic structure of surface defects and their influence on the adsorption of different species, the effect of replacing oxygen with dopants, notably nitrogen, and the role of defect and impurity states as electron and hole trapping sites.