

# Annabella Selloni

*Department of Chemistry, Princeton University,  
Princeton/USA*

**Tuesday, 23<sup>rd</sup> May 2017, 13:30 s.t.**

TU Wien, Freihaus

1040 Wien, Wiedner Hauptstraße 8-10

Yellow Tower „B“, 1<sup>st</sup> floor, Fachgruppenraum Physik  
(gegenüber Mensa)



## Photocatalysis on TiO<sub>2</sub>: insights from simulations

I shall present recent applications of first principles electronic structure calculations and molecular dynamics simulations to understand materials properties and reaction mechanisms in TiO<sub>2</sub>-based heterogeneous photocatalysis. Examples will focus on the structure and reactivity of anatase TiO<sub>2</sub> aqueous interfaces, the behavior of charge carriers at the interface, and the formation and structure of so-called black TiO<sub>2</sub>, a promising functional material capable to absorb the whole spectrum of visible light.

All interested colleagues are welcome to this seminar lecture (45 min. presentation followed by discussion)

Friedrich Aumayr  
(LVA-Leiter)

Ulrike Diebold  
(Seminar Chair)