Contribution ID: **214** Type: **invited talk**

# Electron Dynamics in TiO2 Nanoparticles Study by High Repetition Rate Laser Pump / X-ray Probe Technique

*Thursday, 19 September 2013 16:35 (15 minutes)*

Electron migration and surface trapping are crucial in applications such as photocatalysis and solar energy conversion. Indeed for the former, the migration of charge carriers to the surface, where they can react with species adsorbed onto it, is the most important step.

To address the issue of charge migration, we performed ps time resolved X-ray absorption spectroscopy at the Ti K-edge on TiO2 anatase nanoparticles suspension, using our recently developed high repetition rate data acquisition scheme [1]. After exciting electrons across the band gap at 355 nm, the transient spectrum (excited –ground state sample) at 100 ps clearly shows a localization of the electron at reduced Ti3+ centres that are coordination-unsaturated (i.e. tetra- or pentacoordinated, as opposed to hexacoordinated for the bulk). These unsaturated coordination sites predominantly occur at the surface due to truncation effects [2].

We found that the reduced centres, generated within the 70 ps width of the probe pulse, decay typically on two time scales, which we attribute to tetra- and penta-coordinated sites that are promptly populated, as opposed to a cascade mechanism from shallow to deep traps [3].
Similar results were obtained upon injection of an electron into the conduction band from an adsorbed Ruthenium dye (N719, as in dye-sensitized solar cells) excited at 532 nm. This implies that whichever way the electron is delivered to the CB, its ultimate trapping sites are identical.

[1] F. Lima et al., Rev. Sci. Instrum. 2011, 82, 063111.
[2] P.K. Naicker et al., J. Phys. Chem. B, 2005, 109, 15243.
[3] Y. Tamaki et al., J. Phys. Chem. C 2009, 113, 11741.

**Primary author:** Mrs RITTMANN-FRANK, Mercedes Hannelore (Laboratoire de Spectroscopie Ultrarapide, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland)

**Co-authors:** Dr LÜBCKE, Andrea (Laboratoire de Spectroscopie Ultrarapide, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland); Dr MILNE, Chris (SwissFEL, Paul Scherrer Institut, Villigen, Switzerland); Mr SANTOMAURO, Fabio Giacomo (Laboratoire de Spectroscopie Ultrarapide, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland); RITTMANN, Jochen (Laboratoire de Spectroscopie Ultrarapide, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland); Ms SILATANI, Mahsa (Laboratoire de Spectroscopie Ultrarapide, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland); Prof. CHERGUI, Majed (Laboratoire de Spectroscopie Ultrarapide, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland); Mr REINHARD, Marco (Laboratoire de Spectroscopie Ultrarapide, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland); Dr ABELA, Rafael (SwissFEL, Paul Scherrer Institut, Villigen, Switzerland); Dr PENFOLD, Thomas James (Laboratoire de Spectroscopie Ultrarapide, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland)

**Presenter:** Mrs RITTMANN-FRANK, Mercedes Hannelore (Laboratoire de Spectroscopie Ultrarapide, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland)

**Session Classification:** Functional Materials