Ultrafast charge carrier dynamics in solar materials: X-ray studies

Transition metal oxides (TiO_2, ZnO, NiO) are large gap (> 3eV) semiconductors that have been studied for many years now due to their applications in solar energy conversion and in photocatalysis. In recent years, perovskites have attracted huge interest as novel solar materials. The applications of these materials depend on the generation of charge carriers (electrons and holes) and on their subsequent evolution as excitons or polarons, and eventually their localization either as self-trapped excitons or at defects. While several ultrafast THz, infrared and visible probe studies have been performed on the electron dynamics in the conduction band (CB) of the material, these cannot distinguish free from localized electrons, and they miss to probe the hole dynamics in the valence band (VB). Using time-resolved X-ray spectroscopy pioneered by my group, we will present the following results: i) By ps, and fs X-ray absorption spectroscopy, we identified the trapping sites and times in anatase TiO_2; ii) using a combination of ps and fs XAS and Resonant Inelastic X-ray Scattering (RIXS), we identified the dynamics of hole trapping in ZnO; iii) we have probed the charge carrier dynamics in perovskites with element selectivity, establishing the nature of the exciton in these materials.