

Monitoring photocatalysis at the TiO₂ surface in real time using soft X-ray photoemission spectroscopy

Michael Wagstaffe, Adrian Dominguez-Castro, Lukas Wenthaus, Thomas Frauenheim, Andreas Stierle, and Heshmat Noei

DESY NanoLab, Hamberg, Germany

An acute understanding of photocatalytic reaction dynamics on metal oxides is crucial for the efficient development of technology used for self-cleaning surfaces and for air and water purification. By utilizing femtosecond X-ray laser pulses synchronized with an optical laser (1.6 eV) at FLASH we were able to directly follow the reaction dynamics during photocatalysis at the surface of anatase TiO₂(101) for two different prototypical systems; CO/O₂/TiO₂ and H₂O/TiO₂. This technique allowed us to monitor the dynamics of reaction product formation with high chemical sensitivity and in real time. Our time-resolved soft X-ray photoemission spectroscopy results are combined with theoretical calculations to provide crucial insight concerning reaction mechanisms and dynamics. Furthermore, the observation of subtle transient core level shifts provides information on interfacial charge transfer during the initial steps of the reaction immediately following the formation of the photogenerated charge carriers.