Report from abroad travel

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3. **Travel purpose:** Participation in DESY Photon Science/*XFEL* Users Meeting conference
4. **Country and area target:** DESY , Hamburg Germany
5. **Duration of travel:** 24-27.01.2017
6. **The task / achievement:**

The purpose of this travel was to participant *in* DESY Photon Science/*XFEL* Users Meeting conference, that took place at DESY in Hamburg, Germany. At the conference, the poster was presented with title: '*Doping effect on electronic structure of TiO2'* (The poster is attached to this report). TiO_2 is the most commonly used photocatalyst but it requires excitation with UV light due to its wide band gap (3.2 eV). A common strategy to improve visible light absorption is to reduce the band gap energy by doping with 3d elements, which shifts the conduction band downwards in energy and/or light elements such as N, C and S able to shift the valence band upwards in energy. The poster contained experimental results of measurement of the X-ray emission and absorption of chromium and nitrogen doped titanium dioxide, and they are compared with theoretical calculations for densities of states.

The calculated density of states for Cr-doped TiO_2 reveals twofold influence on electronic state composition. First the Ti 3d-band is slightly damped in intensity by about 5%, but keep the doublet d-band structure as in case of pure TiO_2. Secondly, a new electronic orbital is introduced on the low energy side of unoccupied electronic states that corresponds to Cr d-band. Based on density of states functions, we calculated pre-edge absorption spectra, which takes into account the excitation probabilities of 1s core-electron. The experimental data shows two-fold effect induced by N-doping. XAS spectrum exhibits slight dumping of first pre-edge structure at energy of 4966eV, but no shift on band positions is detected. For XES measurements, we observe shift of valence-to-core feature to higher energies indicating band gap narrowing. In order to confirm this observation, we calculate N-doping effects on density of states of TiO_2. The computations, shows that indeed N-2p band is introduced on high energy side of valence states of TiO_2 structure.

Thanks to the participation of DESY Photon Science / XFEL Users Meeting conference we noticed new opportunities experiments conducted by our research. This knowledge will undoubtedly help to achieve the intended purpose of our research.

Participation and poster itself was related to project SonataBis no. 622033.

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Date and signatures