Time-resolved X-ray Absorption Spectroscopy of Copper Zinc Tin Sulfide Nanoparticles

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Photovoltaic processes of the earth abundant and non-toxic Cu_2ZnSnS_4 (CZTS) absorber material in 3. generation solar cells can be investigated by time resolved X-ray absorption spectroscopy (TR-XAS) using a synchrotron-based X-ray source and synchronized laser excitation (pump-probe method). Photovoltaic materials require efficient separation of photocarriers and charge mobility, but in CZTS, nanometer scale charge carrier localization has been observed to take place within the first 2 ps after excitation. Localization reduces mobility of charges and it is therefore important to know on what atoms these localizations occur in order to improve the efficiency of the CZTS absorber. We have investigated the carrier localization using pump-probe X-ray absorption spectroscopy (XAS) to track both the oxidation state of Cu and Zn atoms and their local bonding environments at the K-edges of the two metals – 8979 and 9659 eV for Cu and Zn, respectively. In addition, XAS also allow us to investigate the degree of Cu-Zn disorder in the material – the importance of which is still debated by researchers in this field. The investigated CZTS stabilized as a nanoparticle (NP) ink was used as a model system, which is also applicable for low-cost up-scaling of solar cells.