**XRD total scattering of the CZTS nanoparticle absorber layer for the thin film solar cells**

Joanna Symonowicz1\*, Kirsten M. Ø. Jensen2, Sara L. J. Engberg3, Stela Canulescu3

*1 Niels Bohr Institute, University of Copenhagen; 2 Department of Chemistry, University of Copenhagen; 3 Department of Photonics Engineering, Technical University of Denmark*

\*Corresponding author: joanna@symonowicz.pl

Cu2ZnSnS4 (CZTS) thin film solar cells are cheap, non-toxic and present an efficiency up to 9,2% [1]. They can be easily manufactured by the deposition of the nanoparticle ink as a thin film followed by a thermal treatment to obtain large grains [2]. Therefore, CZTS has the potential to revolutionize the solar energy market.

However, to commercialize CZTS nanoparticle thin films, the efficiency issues must yet be resolved. In order to do so, it is vital to understand in detail their nanoscale atomic structure. CZTS crystallize in the kesterite structure, where Cu and Zn is distributed between the cation sites in the structure. The cation distribution affects the properties of the CZTS nanoparticles.

Here, we use the hot-injection synthesis method to prepare CZTS nanoparticles of different compositions. Information on the atomic structure is obtained by combining Rietveld refinement of Powder X-ray Diffraction data with X-ray total scattering with Pair Distribution Function analysis. Powder neutron diffraction will furthermore allow characterization of the cation disorder on the metal sites in the kesterite structure. The nanoparticle ink is also characterized by XRD, EDS, and Raman spectroscopy in order to fully detect possible secondary phases and characterize the CZTS phase.

[1] T. Kato, H. Hiroi, N. Sakai, S. Muraoka, H. Sugimoto; 27th EU PVSEC (2012)

[2] N. Mirbagheri at al., Nanotechnology 27 (2016), 185603 (8pp)