Poster Presentation

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Interplay between off-stoichiometry and intrinsic point defects in compound semiconductors

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The sun provides earth with a staggering amount of energy, but if solar energy is to become a practical alternative to fossil fuels, there must be an efficient way to convert photons into electricity. Photovoltaics (PV) has developed into a mature technology during recent past – thin film PV is an emerging alternative technology because of short energy payback time and minimum use of high purity materials, addressing the urgent need for cost-competitive renewable energy technologies. Compound semiconductors, like chalcopyrite type Cu(In,Ga)(Se,S)2 (CIGSe), are the most advanced and most efficient absorber materials. Such solar cells show present record lab efficiencies of >22% [1]. Since the availability of indium is an object of concern regarding the large scale production of solar cells, its replacement with Zn and Sn is beneficial in this sense. Compounds like Cu2ZnSn(S,Se)4 (CZTS, CZTSe) are an alternative. One of the reasons for the success of CIGSe based thin film solar cells is the remarkable flexibility of its chalcopyrite type crystal structure. This flexibility is a key also for the quaternary kesterite type compounds CZTS,Se because the thin film growth is in fact a non-equilibrium process. The absorber layers of high efficient solar cells exhibits an overall off-stoichiometric composition, thus the existence of intrinsic point defects is strongly correlated with the chemical potential and therefore dependent on the composition of the material. These structural defects influence the electronic properties of the final device sensitively. A high density of bulk defects and structural disorder (Cu/Zn disorder) will cause an extreme band tailing which could account for a significant part of the open circuit voltage (Voc) loss, the main limitation for the performance of CZTS,Se-based PV devices. Our research focuses on the correlation between off-stoichiometry, point defects and physical properties of kesterites. We have demonstrated, that kesterite type CZTSe can self-adapt to Cu-poor and Cu-rich compositions without any structural change except the cation distribution [2]. The ability to accept deviations from stoichiometry, which can be categorized in off-stoichiometry types (A-L), is correlated to a Cu/Zn disorder (see figure) and the formation of intrinsic point defects. Using synchrotron X-ray and neutron diffraction data in a complementary approach we have established correlations between stoichiometry deviations and occurring intrinsic point defects (type and concentration) in CZTS,Se kesterites. We were able to show for the first time quantitatively that the Cu/Zn disorder in kesterites causes shifts in the energy band gap [3] giving raise to band tailing a possible performance limiting parameter for thin film solar cell devices based on kesterite-type absorber layers.
The presentation will underline the role of crystallographic materials research to provide the basis for the understanding of structure-property relations of energy materials.

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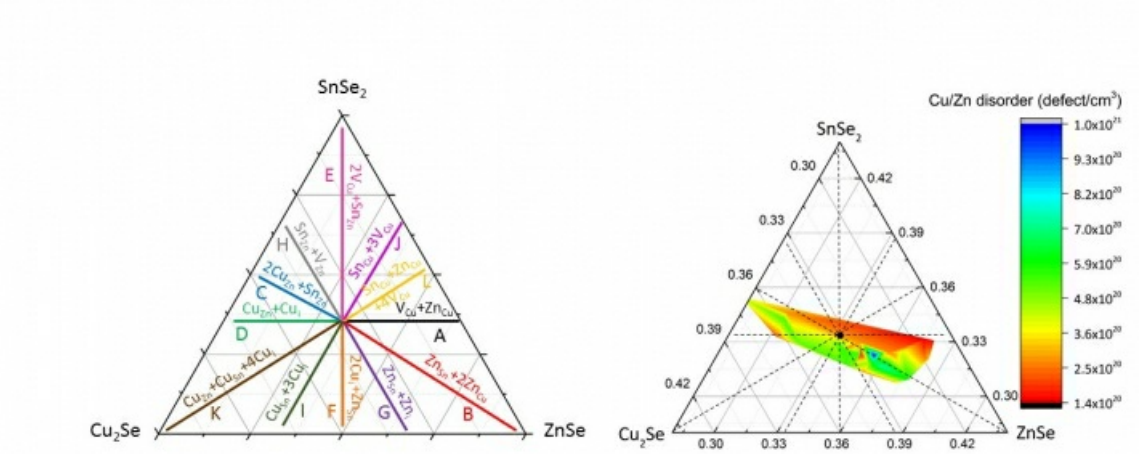

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