

## EMIL – Energy conversion devices illuminated by soft and hard x-rays

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The complexity of energy conversion devices, which are often comprised of a multitude of layers, interfaces, surfaces, elements, impurities, etc., make it both difficult and crucial to characterize and understand the chemical and electronic structure of each component and their interactions. It is demonstrated that the combination of different soft and hard x-ray spectroscopies is an extraordinary method for illuminating the chemical and electronic material characteristics from many different perspectives, ultimately resulting in a comprehensive picture of these properties.

This presentation will **first** focus on our recent progress in the characterization of thin-film solar cell layer stacks. In detail, we will use our studies on the impact of different post-deposition treatments (PDT) on the chemical and electronic surface structure of high-efficiency Cu(In,Ga)Se<sub>2</sub> (CIGSe) thin-film solar cell absorbers to demonstrate the capabilities of the analysis approach outlined above. As described in detail in Refs. [1-3], a NaF/KF PDT has recently led to new record efficiencies of CIGSe thin film solar cells. Alkali-free CIGSe, NaF-PDT CIGSe, and NaF/KF-PDT CIGSe absorbers grown by low-temperature coevaporation were compared and contrasted. Using a combination of depth-sensitive soft and hard x-ray photoelectron spectroscopy as well as soft x-ray absorption and emission spectroscopy, a detailed insight into the chemical structure of the CIGSe surface and how it changes upon different PDTs has been gained. We find that the alkali-free and NaF-PDT CIGSe surfaces both display the well-known Cu-poor CIGSe chemical surface structure. The NaF/KF-PDT, however, leads to the formation of a bilayer structure in which a K-In-Se species covers the CIGSe compound that, in composition, is identical to the chalcopyrite structure of the alkali-free and NaF-PDT absorber. Furthermore, for all samples we find the position of the valence band maximum shifts away from the Fermi level with increasing surface sensitivity, with this effect being most pronounced for the NaF/KF-PDT CIGSe sample. In combination with additional inverse photoemission measurements, we find the surface band gap ( $E_g^{\text{Surf}}$ ) for the NaF/KF-PDT absorber (2.52 eV) significantly enlarged compared to the CIGSe bulk band gap (1.15-1.20 eV) and to the  $E_g^{\text{Surf}}$  of 1.61 eV found for an absorber treated with NaF only. The observed electronic structure changes are in agreement with the revealed chemical surface properties and can be linked to the recent breakthroughs in CIGSe device efficiencies.

The **second** part of the presentation will focus on the newly setup Energy Materials In-Situ Laboratory Berlin (EMIL) and its analytical and deposition capabilities. EMIL is a new multi-user large-scale research platform located at HZB's synchrotron radiation source BESSY II. With a canted double undulator

system in the BESSY II storage ring, the EMIL analytics has access to x-rays ranging from 80 eV up to 10 keV. EMIL is a “joint venture” of the Max Planck Society and the HZB. While the research focus of the Max Planck Society within EMIL is on catalysis, the HZB concentrates on energy materials research. For that purpose, a variety of industry-relevant synthesis and preparation tools are connected to HZB’s analysis chambers (which combine various complementary x-ray and electron spectroscopies) via fully automated ultra-high vacuum (UHV) transfer allowing easy *in-system* characterization of materials and layer-stacks. In order to bridge the pressure gap between UHV-based analytics and operational conditions, in particular in view of dye-sensitized solar cells, (photo)electrochemical water splitting, electrochemical energy storage, etc., a route to *true operando* studies under *atmospheric* conditions will also be presented.

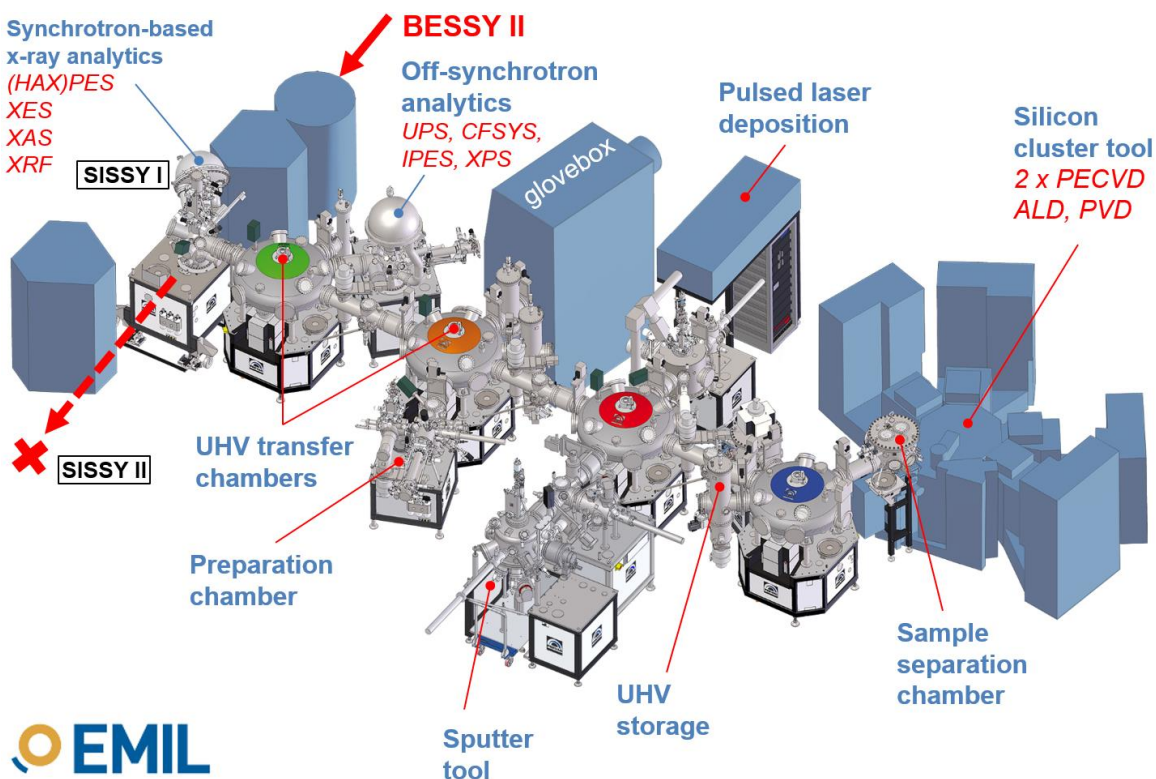


Fig. 1 Schematic presentation of the current status of the combination of analysis and deposition tools for HZB’s energy materials research at EMIL.

#### References

- [1] Chirilă, A.; Reinhard, P.; Pianezzi, F.; Bloesch, P.; Uhl, A. R.; Fella, C.; Kranz, L.; Keller, D.; Gretener, C.; Hagendorfer, H.; Jaeger, D.; Erni, R.; Nishiwaki, S.; Buecheler, S.; Tiwari, A. N. *Potassium induced surface modification of Cu(In,Ga)Se<sub>2</sub> thin films for high efficiency solar cells*. *Nat. Mater.* 2013, **12**, 1107–1111.
- [2] Handick, E.; Reinhard, P.; Alsmeyer, J.-H.; Köhler, L.; Pianezzi, F.; Krause, S.; Gorgoi, M.; Ikenaga, E.; Koch, N.; Wilks, R. G.; Buecheler, S.; Tiwari, A. N.; Bär, M. *Potassium Postdeposition Treatment-Induced Band Gap Widening at Cu(In,Ga)Se<sub>2</sub> Surfaces – Reason for Performance Leap?* *ACS Appl. Mater. Interfaces* 2015, **7**, 27414–27420.
- [3] Handick, E.; Reinhard, P.; Wilks, R. G.; Pianezzi, F.; Kunze, T.; Kreikemeyer-Lorenzo, D.; Weinhardt, L.; Blum, M.; Yang, W.; Gorgoi, M.; Ikenaga, E.; Gerlach, D.; Ueda, S.; Yamashita, Y.; Chikyow, T.; Heske, C.; Buecheler, S.; Tiwari, A. N.; Bär, M. *Potassium Postdeposition Treatment-Induced Band Gap Widening at Cu(In,Ga)Se<sub>2</sub> Surfaces – Reason for Performance Leap?* *ACS Appl. Mater. Interfaces* 2017, **9**, 3581–3589.