Abstract: We present an alternative explanation for the open circuit voltage (OCV) deficit in CuInZnSnS3 (CZTS). Using a method based on tools available in the Atomistix ToolKit (ATK) software package, we have studied the electronic structure at the interface between CZTS and CdS in detail. Here, we have identified a shallow state localized at the interface. When included in device level simulations, such a state leads to significant deterioration of the OCV, and when this is taken into account, we can quantitatively reproduce measurements on state-of-the-art CZTS solar cells. This shows how parameters needed for device characterization can be extracted from atomistic device simulations and how the interplay between atomistic and device level simulations can be a powerful tool in characterizing the thin-film solar cell devices of the future.

Solar Cell: CZTS/CdS Interface

The full solar cell consists of several layers of materials, with key mechanisms related to each of them, as well as the interfaces between them. In this work, we focus on the interface between CZTS(CIS) and CdS, which has been shown to be important for this class of materials.

Modeling the Device with DPT-NEG

We use the DPT-NEG method implemented in the Atomistix ToolKit (ATK) software package to calculate the band structure of an interface between two semi-infinite bulk materials. This allows us to treat the interface much more realistically than previous works, meaning that the interface was infinitely thick. In our case, there is only the one interface in the system, which is comprised of both bulk regions of CZTS and CdS.

Calculating Circuit Voltage

In order to find the macroscopic effect of these interface states, we performed device-level simulations using the SCAPS software. As expected, this showed that the open-circuit voltage was significantly lowered by the interface states, and the value at room temperature, 720 mV, is very close to the experimental record of 760 mV. This interface state is also expected to lower the expected efficiency for even the best CZTS/CdS solar cells.

Results

After further analysis, it was determined that ZnS would be a good candidate for a buffer material which could reduce the interface states, and thereby increase the maximum efficiency of the solar cell. The figure shows that the ZnS interface state is indeed gone when CdS is exchanged with ZnS.

Conclusions

- We have presented a multi-scale framework for simulating Photovoltaics.
- Device parameters, such as band offsets, are calculated from first principles using DPT-NEG with the +1 correction and included in a drift-diffusion device simulator - in this case the SCAPS-1D software.
- Applying this approach, we obtain quantitative results for a CZTS/CdS device, which shows the interplay between the gap and the valence band edge. They can be included in the drift-diffusion model, which reveals the importance of interface states.

References