ENERGY BAND ALIGNMENT AT OXIDE SEMICONDUCTOR INTERFACES

A. Klein, F. Säuberlich, G. Liu, S. Tiefenbacher, W. Jaegermann

Institute of Materials Science, Darmstadt University of Technology
Petersenstrasse 23, 64287 Darmstadt, Germany,
phone +49-6151166354, FAX +49-6151166308, e-mail aklein@surface.tu-darmstadt.de

Transparent conductive oxides as ZnO, ITO, SnO_2 and TiO_2 are essential parts of all thin film solar cells. In general, the solar cell conversion efficiencies are strongly affected by the interfacial barrier heights. It is therefore important to understand not only the dependencies of the optical and electrical properties of TCO's, but also of their surfaces and interfaces.
The barrier heights have been determined for a number of oxide/semiconductor combinations using photoelectron spectroscopy. Experimentally determined energy band diagrams are shown in Fig. 1. There are quite small conduction band offsets for the interfaces between In_2O_3, SnO_2 and ZnO with II-VI semiconductors CdS and CdTe, resulting in small barriers for electron transport. This is desirable for CdTe and CIGS solar cell applications. The vacuum levels, however, exhibit very large steps at the interfaces, which is the result of an electron transfer from the oxide to the II-VI semiconductor. Large interface dipoles are also observed for TiO_2 / chalcogenide (CdTe, Cu_2S) interfaces. Such contacts are interesting for solid-state injection type solar cells. Because of the larger electron affinity of TiO_2 compared to the other TCOs, the band alignment at these interfaces is characterized by a large conduction band offset.

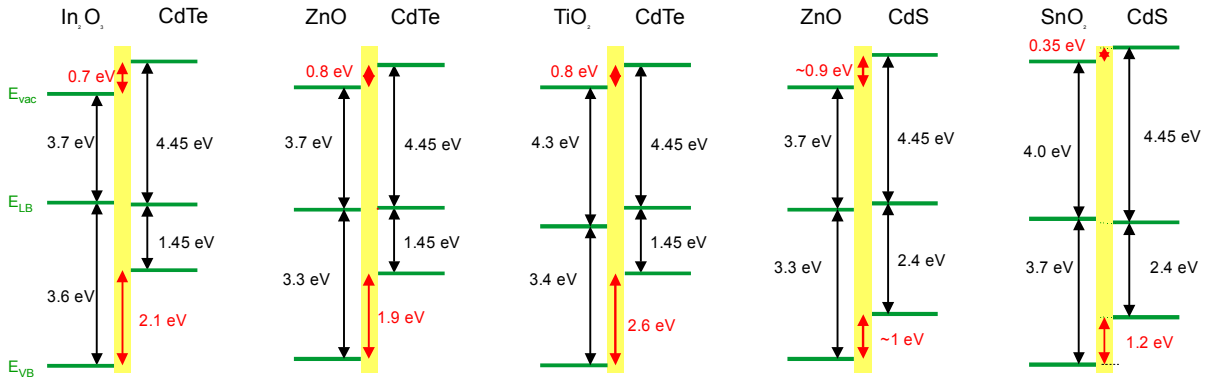

Fig. 1: Experimentally determined energy band diagrams of different TCO / II-VI semiconductor interfaces.

In organic solar cells and dye-sensitized solar cells ITO and TiO_2 are used as electrode material in contact with organic materials. Small interface dipoles of ~0.3 eV are reported for ITO / organic interfaces. They are also oppositely oriented compared to the TCO / II-VI interfaces, which means an electron transfer from the organic material to the ITO.