Band offsets in heterojunction solar cells – a new view on a (very) old story

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Heterojunctions in solar cells are unavoidable, either because of the need for selective contacts or in cases where the absorber cannot be doped sufficiently high or in different types. The conduction band alignment at the electron contact and the valence band alignment at the hole contact are decisive for the functioning of the solar cell. It's been long known that negative bandoffsets (e.g. conduction band of the contact below conduction band of absorber) increase interface recombination and too large positive bandoffsets lead to barriers for the photocurrent [1]. But there are quite a few misconceptions in the literature. And it is interesting to understand why drift-diffusion approximations lead to different current densities than thermionic emission considerations. It is therefore useful to have a detailed look at the models for current transport over barriers. We will demonstrate the concept for sulfide chalcopyrite $Cu(InGa)S_2$ solar cells with different (ZnSn)O buffers. Their bandgap above 1.6eV makes them interesting as top cells in tandem cells [2]. Chalcopyrites have proven their stability in more than a decade of applications in the field. With an (active area) efficiency of 16.1% in a cell with a transparent back contact, we can demonstrate first efficient tandem cells.

[1] G. B. Turner, R. J. Schwartz, and J. L. Gray, in *20th IEEE PV Specialist Conference*, edited by IEEE (IEEE, Las Vegas, 1988), p. 1457.
[2] D. Adeleye *et al.*, Small **21**, 2405221 (2025).