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Band offsets at the crystalline / hydrogenated amorphous silicon interface from first-principles EBRAHIM HAZRATI, KAROL JAROLIMEK, GILLES A. DE WIJS, Roadbed University, Nijmegen, The Netherlands, INSTITUTE FOR MOLECULES AND MATERIALS TEAM — The heterojunction formed between crystalline silicon (c-Si) and hydrogenated amorphous silicon (a-Si:H) is a key component of a new type of high-efficiency silicon solar cell. Since a-Si:H has a larger band gap than c-Si, band offsets are formed at the interface. A band offset at the minority carrier band will mitigate recombination and lead to an increased efficiency. Experimental values of band offsets scatter in a broad range. However, a recent meta-analysis of the results (W. van Sark et al.pp. 405, Springer 2012) gives a larger valence offset (0.40 eV) than the conduction offset (0.15 eV). In light of the conflicting reports our goal is to calculate the band offsets at the c-Si/a-Si:H interface from first-principles. We have prepared several atomistic models of the interface. The crystalline part is terminated with (111) surfaces on both sides. The amorphous structure is generated by simulating an annealing process at 1100 K, with DFT molecular dynamics. Once the atomistic is ready it can be used to calculate the electronic structure of the interface. Our preliminary results show that the valence offset is larger than the conduction band offset.

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