FIRST-PRINCIPLES ANALYSIS OF THE INTERMEDIATE BAND IN Fe-DOPED $CuGaS_2$

J. Koskelo, J. Hashemi, S. Huotari, and M. Hakala

Department of Physics, P.O. Box 64, FIN-00014 University of Helsinki, Finland
email: jaakko.koskelo@helsinki.fi

Intermediate-band (IB) solar cells [1] are potential candidates for next-generation high-performance photovoltaics. An IB is an additional energy band located between the valence and conduction bands that can improve solar-cell efficiency by enabling optical transitions that allow to exploit larger portion of the solar spectrum. IB solar-cell absorbers can be produced by doping semiconductors with metal impurities. The gallite $CuGaS_2$ is a promising host semiconductor, and Fe-doping has been shown to induce IBs [2].

We investigate the electronic structure, dopant configuration, and optical properties of $CuGa_{1-x}S_2Fe_x$ by performing calculations [3] using a hybrid exchange-correlation functional. We show that the Fe dopants tend to cluster and prefer antiferromagnetic ordering. We find unoccupied IBs between 1.6 and 1.9 eV above the valence band maximum. We discuss the similarities and differences of our theoretical optical absorption spectra compared to experimental one [2] and implications on the assignment of spectral features. Furthermore, we study the effect of n-type co-doping. We find that the IB can be partially filled with small enough electron concentrations, but large concentrations lead to shift of the occupied part of the IB on top of the valence band.

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[2] B. Marsen, S. Klemz, T. Unold, and H.-W. Schock, Progr. Photovoltaics: Res. Appl. **20**, 625 (2012).
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