

Transition metals doped I-III-VI₂ compounds for advanced photovoltaics

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CuInSe₂ and other chalcopyrite compounds have long demonstrated their potential as photovoltaic materials with record efficiencies on thin film cells of 19.5% (lab sized cells) and 13 % (manufactured modules). Besides PV performance, these materials have displayed an exceptional tolerance to defects and impurities.

The chemistry of this family of compounds enables insertion of elements capable of imparting them new functionalities without altering their good electronic properties. This could possibly lead to new materials with improved photovoltaic properties. *Ab initio* calculations have already provided new insights on their electronic structure and their intrinsic defects [1, 2].

The introduction of levels in one of the spin character band may lead to new conversion scheme and improved performance [3]. Magnetic transition metals can be candidate for such systems and their effect on the electronic structure has been investigated by *ab initio* calculations. Alternatively, magnetic impurities may lead to some interesting properties related to spintronic applications by the way they can affect the band structure and the density of states.

For instance, cases will be presented where magnetic impurities could allow for the design of materials with a potential photovoltaic conversion efficiency up to 60%, i.e. twice the potential of current materials actually used in photovoltaic devices. Different 3d transition metals (Fe, Mn, Co, ...) have been substituted on I and III sites in CuGaS₂. According to the transition metal chosen ferro or antiferro magnetic coupling can be present. Depending the transition metals potential degradation or improvement of the photovoltaic properties will be discussed.

[1] S.B. Zhang, S.H. Wei, A. Zunger, and H. Katayama-Yoshida, Phys. Rev. B **57** (1998) 9642

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[3] J. M. Raulot, C. Domain, J.F. Guillemoles, to appear in Phys. Rev. B