Multiferroic materials with tailored electronic properties for efficient light harvesting applied to solar cells

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Although Si-based solar cells are widely used to convert light into electric current, their efficiency reached already 25%, close to the thoretical Shockley-Queisser limit which is about 30%.[1] In this context, alternative materials are intensively studied in order to further improve the performances of solar cells. For this purpose different strategies can be adopted. One strategy already tested takes advantage of the down-shifting or down-conversion phenomena that can limit the thermal losses and increase the number of photons that can be converted into electric current. For this purpose a large bandgap rare-earth doped oxide layer is added on the top of the solar cells. The efficiency improvement is however modest (less than 1%) mainly because of the reduced energy transfer efficiency from the host to the rare earth ions. Another way to improve the efficiency of solar cells could result from the use of *ferroelectric oxides* as photon absorber. Besides their chemical stability when compared to hybrid perovskites, ferroelectric oxide based solar cells do not need a p-n junction as in conventional photovoltaic devices since the internal electric polarization is now responsible for electron-hole separation. The main challenge is to develop ferroelectric oxide materials with an appropriate bandgap with respect to the solar spectrum. Such oxide could be the Bi_2FeCrO_6 (BFCO) double perovskite. In epitaxial films, we suceeded to modulate the gap between 1.9 and 2.6 eV by controlling the growth conditions which influences on the Fe/Cr order.[2] However, this order remains overall very poor due to the similar ionic radius and valences of the Fe and Cr in the BFCO structure. Band structure calculations confirmed our experimental results. The ferroelectric properties were studied using the piezoresponse force microscopy (PFM) and the ferroelectric character of the material was clearly demonstrated. Test PV devices based of BFCO were fabricated but their efficiency remained small mainly due to the large Fe-Cr disorder and to the low shot-circuit current. However, other authors managed improving the Fe-Cr order. The gap can be reduced down to 1.4 eV and the efficiency of solar cells integrating such layers increased to 3 and 8% for single- and multi-junctions cells, respectively.[3]

In this context, the aim of this work is to modulate the electrical properties of BFCO either by modulating the deposition conditions in order to improve the Fe-Cr order, or by doping at the A (Sn, Sb) and B/B' (Ni, Mn, Cr) sites. This should allow modulating the gap, carrier concentration and mobility with strong impact on the cell efficiency (light absorbtion, J_{sc}, V_{oc}). Finally, such films may have a positive impact on other subjects developed at IPCMS such the ones oriented towards data storage using multiferroic materials.

We look for a dynamic cadidate (master level), with strong personal motivation and solid background in physics, solid state chemistry or materials science. Good knowledge of English is desirable. He/she will be involved in the deposition of thin films, structural, and transport characterisation, as well as in the fabrication and testing of solar cells. IPCMS will actively promote the career of a successful PhD candidate within the relevant research communities through the participation in national and international conferences.

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[1] W. Shockley and H.J. Queisser, J. Appl. Phys. 32, 510 (1961).
[2] A. Quattropani, D. Stoeffler, T. Fix, G. Schmerber, M. Lenertz, G. Versini, J.L. Rehspringer, A. Slaoui, A. Dinia, and S. Colis, *J. Phys. Chem. C* 122, 1070 (2018).
[3] R. Nechache, C. Harnagea, S. Li, L. Cardenas, W. Huang, J. Chakrabartty, and F. Rosei, Nature Photonics 9, 61 (2014).