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Magnetoelectic multiferroic superlattices and interfaces: Designing spintronic materials from first principles[1]

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The research challenges of the near and far future in electronics focus on the quest for new materials and novel device concepts to achieve low energy consumption, increased reliability and high device density. These can be obtained by designing active elements and interconnects whose operating principle is not (only) based on the electron charge but on the spin degree of freedom of the electron. The nanoscopic size of the materials calls for atomistic and parameter free (*ab initio*) simulations, which have proven to be crucial in achieving the necessary accuracy and predictive power. Materials which present a coupling between ferroelectricity and magnetism, i.e. magnetoelectric (ME) multiferroics, have been proposed as fundamental building blocks for spintronic devices [1]. However ferroelectricity and magnetism are often exclusive or weakly coupled in bulk. In this talk, we will discuss how superlattices of perovskites can be designed from first principles to achieve strongly coupled ME and, hence, achieve control the weak magnetization via an electric field [2]. Most important, advanced epitaxial techniques allow one to actually grow such magnetoelectric superlattices [3]. Another route to optimize spintronic devices is to exploit the unique electronic and transport properties of Carbon-based nanomaterials [4]. The latter present spin diffusion lengths up to 100 μm and high electron velocity. However, a large spin diffusion length comes at the price of small Spin Orbit coupling, which limits the possibility of manipulating electrons *via* an external applied field. Further, to achieve graphene-based devices one also needs to open its vanishing electronic gap. We use first principle techniques to show that placing graphene on a ME substrate can overcome these limitations by inducing magnetism and opening an electronic band-gap in the hybrid organic-multiferroic material.

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