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Electric polarization of $Sr_{0.5}Ba_{0.5}MnO_3$: a multiferroic Mott insulator[1]

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Multiferroics, materials which display simultaneous magnetic and ferroelectric orders, are interesting both for their rich physics and for their promising practical applications. The search for multiferroic materials with strong-magnetoelectric coupling is challenging and requires an understanding of how the magnetic order, or more specifically the correlations, influence the electric polarization and vice versa. A calculations of the electric polarization in the paramagnetic (PM) insulating phase of multiferroics is essential to address this mutual influence. Ab inito calculations of the electric polarization are based on the modern theory of polarization, which is a single-electron theory. Thus, a correlation driven insulating state is beyond the scope of this approach. Here we show that combining correlated band structure calculations (DFT+DMFT) with a formula for the electric polarization of interacting insulators, expressed in terms of the full Green and vertex functions, allows for the first time to reliably calculate the polarization in the PM phase. We focus on the Mott insulator $Sr_{0.5}Ba_{0.5}MnO_3$, in which both magnetic and ferroelectric instabilities are related to the Mn ions. We predict a ferroelectric polarization of $\simeq 16.5\ \mu C/cm^2$ in the high temperature paramagnetic phase and recover the measured value of $\simeq 13.3\ \mu C/cm^2$ in the low temperature antiferromagnetic phase. Our calculations reveal that the the driving force behind the ferroelectric distortion comes from the tendency of Mn e_g states to establish a stronger covalency with the surrounding oxygens. This covalency is reduced by correlations, in particular by Hund coupling. On the other hand, the half-filled Mn t_{2g} orbitals give rise to the magnetic ordering which decreases the ionic displacement, hence its contribution to the polarization. For fixed ionic displacement, the magnetic order also slightly decreases the electronic contribution to the electric polarization by partially polarizing the Mn eg orbitals through Hund coupling. Despite this last effect, which would lead to positive magneto-electric coupling, the combination of the two effects gives a negative magneto-electric coupling.

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