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Epitaxially-strained GeTe as a prototype material for a microscopic understanding of bulk Rashba properties

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Relativistic effects are increasingly seen as key ingredients in the burgeoning field of spintronics. Among them, the Rashba effect, in which the spin degeneracy is removed as a consequence of spin-orbit coupling (SOC) in noncentrosymmetric structures, plays a leading role. An interesting subclass of bulk materials lacking inversion symmetry is represented by ferroelectrics, which could in principle allow to bring in a novel functionality through the interplay between ferroelectricity and SOC-induced Rashba spin-splitting (RSS). For such materials, the coupling of RSS with electric polarization opens up a wide range of potential applications in the field of semiconductor spintronics, aiming at an all-electric control of spin transport in novel devices. In this context, many efforts are now given in the search for such multifunctional materials and strain engineering is nowadays regarded as a powerful tool to tune these highly desirable properties.

Using first-principles calculations, we simulated a (111) epitaxially-strained growth and computed the changes in the structural, electronic and magnetic behaviour of GeTe, a ferroelectric material known to also exhibit a wide bulk RSS. Interestingly, our results showed that RSS could not be driven by the sole modification of the ferroelectric polarization and the electronic band gap, as usually believed. Further DFT calculations and the elaboration of a tight-binding model lead to the identification of the main parameters entering the strength of RSS and identify their contribution. This study indicates that the RSS is not only strongly k-dependent, but also very sensitive to the orbital character of the bands around the Fermi level. Our findings highlight the decisive influence of the electronic structure on spin-orbital properties and the need of a deep understanding of these features for each multifunctional material.