An experimental and computational study on the effects of the ferroelectric transition in the electronic structure of SnTe

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In the recent years, the need in modern technologies for new materials with special properties is growing more and more. In this context, interesting candidates for applications lie in ferroelectric materials, in which a distortion of the atomic structure implies a spontaneous electric polarization of the material, switchable and tunable with the application of an electric field.

This work presents an experimental and computational study of the electronic structure of SnTe with angle-resolved photoemission spectroscopy. This semiconductor is particularly interesting because its transition temperature between the ferroelectric and the paraelectric state (for which thermal energy induces an absence of spontaneous polarization) is around 100 K, a temperature easily accessible with photoemission spectroscopy setups. Therefore, our objective is to investigate the electronic structure in the ferroelectric phase and, more importantly, characterize the effects of the phase transition in the electronic structure, which is still unexplored in the literature.

With the help of Density Functional Theory predictions, we analyze our experimental results and present our hypothesis of an order-disorder transition between the ferroelectric and the paraelectric state.

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