Bulk band splitting due to spin-orbit interaction in ferroelectric oxides

Dana Gerogeta Popescu
Lucian D. Filip, Cristina Chirila, Luminita Hrib, Marius A. Husanu
National Institute of Materials Physics, Atomistilor 405 A, 077125 Magurele, Romania
ahusanu@infim.ro

Abstract

Ferroelectricity resulted from off-centering of cations in perovskite oxides breaks the space inversion symmetry. This, in conjunction with the presence of heavy atoms such as Bi in $BiFeO_3$ or Pb in $PbTiO_3$ is a natural ingredient to promote large spin-orbit interaction, accompanied by splitting of the bulk band structure, with well-defined spin orientation.
Our DFT calculations with and without spin-orbit interaction indicate that the valence band maximum of $PbZrTiO_3$ – PZT is featured by spin-split bands. This is decided by comparing calculations perfromed in the ferroelectric state and in an artificial, paralectric and centrosymmetric case.
The theoretical calculations are compared with the experimental band structures, where spin-resolved photoemission is employed to record the spin polarized band structure.
The challanges of resolving the band structure of ferrolectric materials in well-defined ferroelectric state are also discussed.