Highlights

Activity F - Electronic and thermal transport from the nanoscale to the macroscale - 2021

Strain-induced topological phase transition at (111) $SrTiO_3$ -based heterostructure

M. Trama [1,2], V. Cataudella [3,4], C. A. Perroni [3,4]

[1]Physics Department "E.R. Caianiello", Universitá degli studi di Salerno, Via Giovanni Paolo II, 132, I-84084 Fisciano (Sa), Italy
[2]INFN - Sezione di Napoli, Complesso Univ. Monte S. Angelo, I-80126 Napoli, Italy
[3]Physics Department "Ettore Pancini", Universitá degli studi di Napoli "Federico II", Complesso Univ. Monte S. Angelo, I-80126 Napoli, Italy
[4]CNR - SPIN Napoli Unit, Complesso Univ. Monte S. Angelo, Via Cintia, I-80126 Napoli, Italy

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The quasi-two-dimensional electronic gas at the (111) $SrTiO_3$-based heterostructure interfaces is described by a multiband tight-binding model providing electronic bands in agreement at low energies with photoemission experiments. We analyze both the roles of the spin-orbit coupling and of the trigonal crystal-field effects. We point out the presence of a regime with sizable strain where the band structure exhibits a Dirac cone whose features are consistent with ab initio approaches. The combined effect of spin-orbit coupling and trigonal strain gives rise to nontrivial spin and orbital angular momenta patterns in the Brillouin zone and to quantum spin Hall effect by opening a gap at the Dirac cone. The system can switch from a conducting to a topological insulating state via modification of trigonal strain within a parameter range which is estimated to be experimentally achievable.

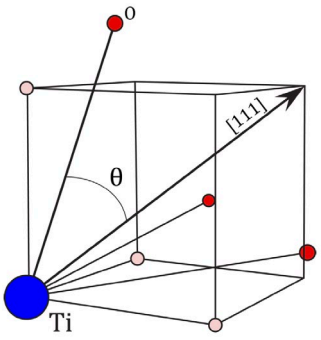

Fig. 1: Cubic structure under a trigonal distortion. The blue sphere is the Ti atom, while the red ones are the O atoms. The pink spheres are the positions of the O atoms in the undistorted structure. The black arrow is the (111) direction. θ represents the distortion angle. When $\theta = arccos(1/\sqrt{3})$ the structure is unstrained; smaller (larger) values of θ lead to dilatation (contraction) along (111) direction.

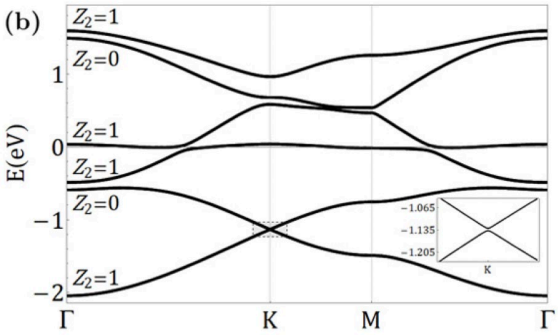

Fig. 2: Electronic band structure of strained (111) $LaAlO_3/SrTIO_3$, exhibiting a Dirac cone at the K point of the Brillouin zone. The inset shows the detail of the Dirac cone. The Z_2 invariant for each band is highlighted: a topological phase is present when the chemical potential is within the band gap at K.