Geometry of the (001) surface and electron dispersion relations of topological IV-VI semiconductors.

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In the electronic structure of topological crystalline insulators (TCI) from the IV-VI semiconductor family there are four Dirac points in the (001) surface Brillouin zone on $\bar{\Gamma} - \bar{X}$ directions. At these points, the energy band gap for surface states is zero due to mirror symmetries with respect to the (110) and ($\bar{1}$10) planes. However, in the experimental works [1-3] it was discovered that there are two pairs of the surface states, one with zero gap and the other with nonzero gap. The opening of the gap suggests that one of the above mirror symmetries is broken. Scanning Tunneling Microscope measurements [2] revealed that the anion and cation sublattices at the surface are displaced relative to each other along the [110] direction by a vector (0.3, 0.3) Å. Such a displacement leads both to breaking the mirror symmetry with respect to the ($\bar{1}$10) plane and the opening of the gap at two Dirac points.

Here, using the local density functional methods we analyse detailed atomic configurations at the (001) surfaces of PbTe, PbSe, SnTe and SnSe. Our results reveal rumpling, *i.e.* relative displacements of anion and cation sublattices in the [001] direction for the first few monolayers, and oscillatory character of interlayer distances between them. Both results are consistent with the previous theoretical and experimental data for the rock salt crystals. However, contrary to the claim of Ref. [2] we do not find any displacements of surface atoms in the (001) plane.

As expected, the rumpling does not open the band gap, because it does not break the mirror symmetry. We also show the dispersion relations for different Sn concentration in $Pb_{1-x}Sn_xSe$ slabs. The chemical disorder leads to the opening of the gap in TCI phase. For Sn concentrations corresponding to Weyl semimetal phase we observe an interval on the $\bar{\Gamma} - \bar{X}$ direction where the gap is vanishingly small.

Calculations are performed using a slab geometry. Optimization of atomic configuration is performed using OpenMX package [4]. Based on an initio results we construct a tight binding hamiltonian for thick slabs. Importantly, to obtain correct results it is necessary to take into account the dependence of tight binding parameters on the distance from the surfaces of the slab.

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[4] see http://www.openmx-square.org