Electronic and thermoelectric properties of bismuth (111) bilayer

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In the following work electronic and thermoelectric properties of bismuth (111) bilayer are investigated using density functional theory (DFT) and tight-binding (TB) method. Bismuth bilayer was among first 2-dimensional systems predicted to exhibit quantum spin Hall effect [1]. Several experiments have confirmed topological nature of edge states in Bi, although there is still on-going debate how robust this effect is with respect to number of layers and type of substrate. It is also known that thermoelectric transport in this material can exhibit new interesting bulk-to-edge corssover [2].

Motivated by those studies, we investigate electronic and thermoelectric properties of thin Bi films. Using sp^3 tight-binding model [3] fitted to our DFT results and Green's functions methods, we check how size and (structural) disorder affects conductance in (111) bismuth bilayers. Then we study thermal transport effects, combining dft and TB methods. We show enhancement of figure of merit in low temperatures and study how it is affected by nanoribbon size, sample disorder, substrate modelled as effective electric field and spatial variations od spin-orbit coupling parameter.

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