**Models for electron transport in the two-dimensional allotropes of bismuth**

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In two-dimensional (2D) materials with honeycomb lattices, such as graphene, spin-orbit coupling is predicted to cause the existence of edge states [1]. The 2D allotropes of bismuth are no exception to this prediction. Although bulk bismuth has been shown to be a topologically trivial semi-metal [2], this material’s 2D allotropes show properties that are topologically non-trivial [3, 4].

More than ten years ago, a tight-binding (TB) model for a bismuth (111) bilayer was proposed by Murakami [3] that is based on an earlier semi-empirical TB model of bulk bismuth [5]. This semi-empirical TB model predicted the existence of edge states in a nanoribbon of (111) bismuth bilayer and, more recently, it has also been used to infer the transport characteristics of a bismuth (111) nanoribbon [4]. For example, Figure 1 shows the band structure of a bismuth (111) nanoribbon computed using this semi-empirical TB model. When using a such a model, however, the atomic structure of the bismuth bilayers cannot be geometry relaxed without further modification to the model that could in turn violate its original ansatz. For the same reason, the electronic structure of bismuthene cannot be computed using this model.



To solve these problems of transferability, we calculate the band structure of the 2D allotropes of bismuth using density-functional theory (DFT) and then develop new TB models of these materials by fitting their energy bands with a basis of maximally-localised Wannier functions. We do this for bismuthene and the (111) and (110) bismuth bilayers.

Our density-functional calculations allow for the atomic structure of the 2D allotropes to be geometry relaxed from bulk. Furthermore, the number of TB parameters in our models have been minimised while not sacrificing the quality of the fits to the band structures from DFT, nor the symmetry of the bases or topologically non-trivial properties of each system. We can therefore be confident that while the resulting Hamiltonians for these nanostructures can be written as sparse matrices, which allow for greater computational tractability, they also accurately capture the physics of each 2D allotrope.

**Figure** Band structure of a bismuth (111) nanoribbon that is 17 nm wide and has armchair edge termination. The bands of two edge states cross the gap between the valence and conduction bands.

Accurate TB models for the 2D allotropes of bismuth are needed to simulate electron transport in these materials, which we do using the non-equilibrium Green’s function formalism. As these 2D allotropes are predicted to be topologically non-trivial, it is essential that TB models reproduce such behaviour.

**References**

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