

Electronic Structure of Impurity Doped Graphene: An Inverse Modelling Approach

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Calculations of the electronic transport properties of nanoscale systems is necessary to understand their possible applications in nanoelectronics and future devices. While there exists a range of techniques for studying transport in regular crystalline materials, there are technical limitations that make most techniques impractical or even unable to model disorder in the material, the exception being the Tight Binding (TB) method.

The reliability and accuracy of these TB calculations relies directly on finding a suitable description of the system (e.g. "hopping" energies, onsite potentials etc.). While several methods exist for doing this, they can be both time-consuming and difficult to fine-tune.

We present a simple and general method for obtaining a TB description of any pristine or disordered nanoscale system using converged numerical quantities, such as formation energy and charge transfer. Although the method is independent of the system, we use graphene as a guinea pig for our method due not only to the mathematical simplicity of its TB model, but also as understanding the controlled doping of graphene to tailor its electronic properties is of great importance to the wider scientific community currently.