A real-space study of random defects in solids : application to disordered graphene

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Abstract

Defects are ubiquitous in solids. They may be formed naturally or artificially. They have profound effect on the electronic structure of solid. So to study the effect of these random defects on the electronic structure of solids is a very important area in the field of material science. Local random defects have been studied by using various methods, but most of the works have been based on supercell method. Long ranged disorder cannot be accessed with these reciprocal space based methods. Here we propose a first principle, parameter free real space method to study the signature of randomly distributed defects through density of states and conducting property calculation. This powerfull technique is applied to graphene with random defects. This real space based technique is general enough so that it can be applied to a whole class of systems where the lattice translational symmetry is not only broken locally but also by extended defects, defect clusters and voids. This method will also allow us to distinguish signature of specific defects and defect clusters.

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