A generalised, tight-binding transport model description for random edge-defected ZGNRs

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The transport properties and magnetisation of edge-defected zig-zag graphene nanoribbons (ZGNRs) have been studied within the Landauer-Büttiker formalism [1] using a generalised tight-binding model that has been shown to be accurate against *ab initio* calculations [2]. The generalised tight-binding model includes up to third nearest-neighbour hopping and a mean-field Hubbard-*U* term, with a single-parameter set for armchair, zigzag and mixed-edge nanoribbon systems [2]. The interplay between the extended hopping, Hubbard-*U* and random edge-disorder on the coherent transport properties has been investigated for small-width ZGNRs of finite device length (Fig. 1a). Second nearest-neighbour hopping and the mean-field Hubbard-*U* have been shown to be essential for reproducing the electronic properties (band-gap and asymmetry) and magnetism in ZGNRs predicted by *ab initio* calculations [2]. Hence this work extends previous studies on ZGNRs that have used only a nearest-neighbour tight-binding model together with random edge-disorder [3-6], or *ab initio* methods to study systematic edge-disorder [7].

Two types of random, edge-disorder were investigated namely, weak-disorder and edge-vacancy defects. Weak-disorder was introduced by perturbing the on-site energy of the edge-atoms by a random amount within the range $\pm|V|$ eV (see also Li *et al*. [3]), whereas edge-vacancy defects were added by random removal of the individual carbon atoms at the edge-sites in a manner that avoids the formation of unrealistic edge-structures (for example Klein defects) (Fig. 1b) [4]. Small-width ZGNR systems were chosen as previous reports have shown that the coherent transport properties of these systems are more sensitive to edge-defects [3]. We calculated ensemble averages for the transport properties using a minimum of 9 randomly generated defected systems in order to ensure good statistics in our results.

Random edge-vacancies are found to decrease the calculated conductance for the ZGNR system (Fig. 2a). Significant differences in the conductance occurs about the Fermi energy (E_F), where the Hubbard-*U* is seen to open up the transport gap. Against the extended model results for the ideal system, the Hubbard-*U* induced gap in the defected system is slightly smaller in width. This *reduction* in width arises from the perturbation obtained in the gap region from the extended hopping terms. Away from E_F there is little difference between the extended model results for systems that are with or without the Hubbard-*U* (Fig. 2a). At higher energies, however, these differences become more significant, and in general, it is shown that the extended model acts to bolster the conductance results.

Random, weak-disorder of the edge-atoms in ZGNR systems results in the formation of a transport gap, which increases in width as a function of the increasing value of the disorder, and has been explained in terms of the onset of Anderson localisation [3-6]. This, however, is not the only mechanism for gap formation in ZGNRs, and therefore we have also been interested to study the interplay between weak-disorder effects and the gap-forming properties of the Hubbard-*U*. Fig. 2(b) shows that Hubbard-*U* effects in the random, weak-disordered system results in a larger transport gap than that of the weakly disordered system described by the hopping terms alone, and that these effects are in fact *additive* resulting in an overall *increase* in the transport gap.

References

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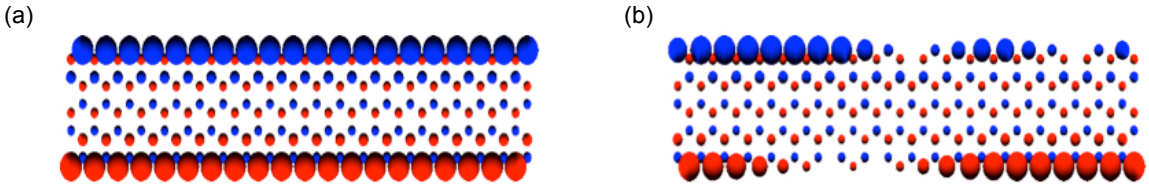

Fig. 1: (a) An ideal ZGNR device showing the dimensions of the ribbon used in this study and (b) a 10% vacancy edge-defected ZGNR device system. Coloured circles correspond to the local spin-polarisation results, where red refers to net spin-up and blue refers to net spin-down.

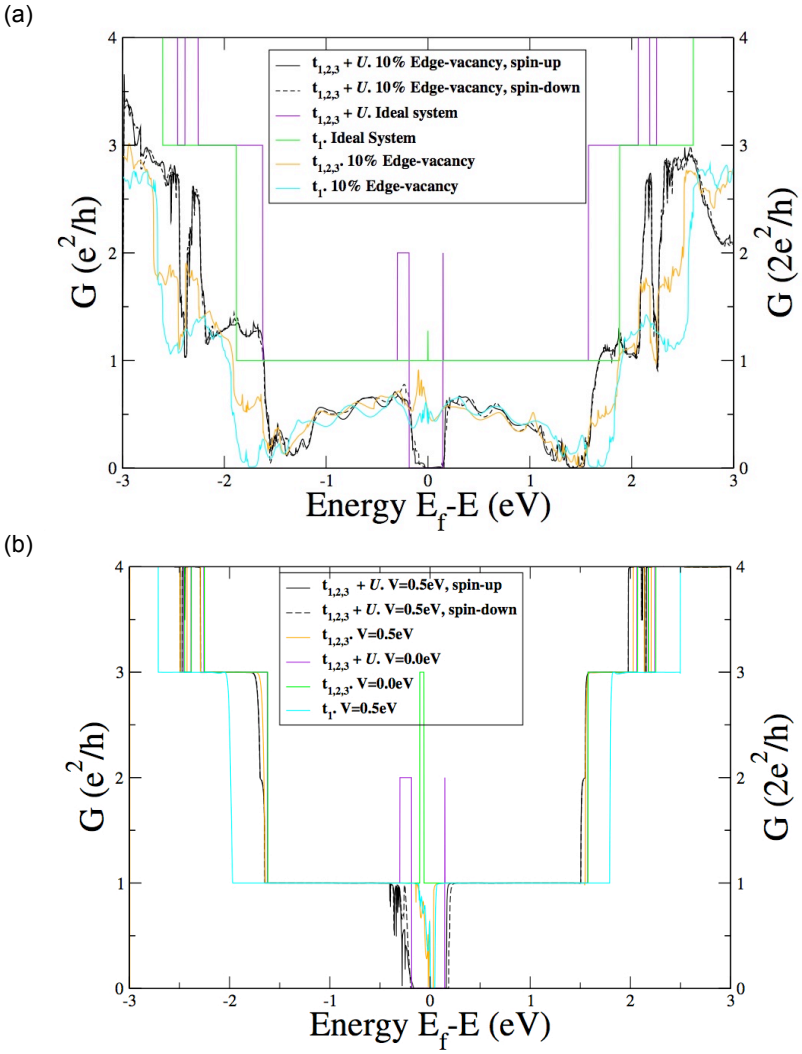

Fig.2: Effect of the mean-field Hubbard-U and extended hopping terms on the transport properties of (a) a 10% random edge-vacancy defected ZGNR and (b) a random, weak-edge disordered ZGNR. Both types of disorder were applied to the ideal ZGNR system shown in Fig 1, with an ensemble average obtained for the results over a minimum of 9 random configurations. Here, $t_{1,2,3}$ (t_1) specifies the range of the nearest-neighbour hopping where 1, 2 and 3 denote first, second and third nearest-neighbour hopping, respectively. The parameters for the generalised, tight-binding model are t_1 = 2.7, t_2 = 0.20, t_3 = 0.18 and U = 2.0 in units of eV. For defected systems with Hubbard-U, solid(dashed) lines correspond to spin-up(down). For all other cases, the results are spin-independent.