Electronic transport in graphene with aggregated hydrogen adatoms

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Abstract

Scattering by resonant impurities, such as covalently bonded hydrogen adatoms, is an important mechanism governing charge conductance in realistic graphene[1]. This type of disorder in 2D systems is known to trigger a non-perturbative Anderson transition for the whole electronic spectrum with an emergence of strongly energy-dependent localization length[2,3]. So far, the effect of resonant scatterers at finite concentrations has been treated as a mere sum of scattering contributions due to individual impurities. However, even the species covalently bonded to graphene are able to diffuse at room temperature, leading to their aggregation due to attractive interactions. We investigate the realistic spatial distribution of hydrogen adatoms on graphene by performing Monte-Carlo simulations based on interaction potentials between adatoms parameterized with the help of first-principles calculations. Hydrogen adatoms show a strong tendency to form small clusters thus ruling out almost entirely the occurrence of isolated adatoms (Fig.1a). The scattering behavior of adatom clusters is very different from single atoms, especially for even-membered clusters that do not show zero-energy resonances[4]. The spectral and transport properties of the constructed models of disordered graphene have been assessed by combining the Landauer-Büttiker approach[5] with the linear response Kernel Polynomial Method (KPM)[6]. A comparison with the case of randomly distributed (non-interacting) adatoms shows that the formation of clusters increases conductance and reduces the extent of the wave-function localization (Fig. 1b-d). Based on the calculated cluster size distributions we introduce a notion of effective concentration of resonant impurities, which provides accurate description of both random and correlated cases.[7]

References

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Figures

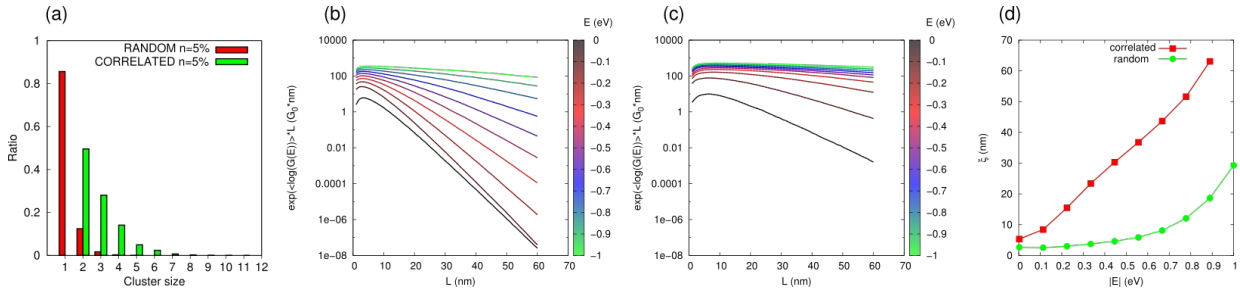

Figure 1: (a) Cluster size distribution for random and correlated hydrogen adatoms at 5% concentration. (b,c) Average conductivity as a function of sample length L calculated for random and aggregated adatoms, respectively, at 5% concentration. (d) Localization length as a function of charge-carrier energy for the two cases.