Towards a realistic model of nanographene – linking theory and experiment

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Accurate modelling of nanographene requires large-scale calculations that take into account realistic device features and system-sizes. Such calculations, however, are mostly beyond the computational reach of density functional theory simulations, and hence more efficient and accurate methods of simulation are actively being sought.

In this work, we have chosen as our starting point, a generalised tight-binding (TB) transport model for nanographene [1], which has been shown to faithfully reproduce density functional theory results (Figs. 1 & 2). The TB model is computationally tractable and can be efficiently scaled to calculate experimentally relevant nanoscale structures. The next step in our model development has been to produce a graphic user interface for graphene (GRUI) (Fig. 3(a)), which has enabled a direct link between theory and experiment using structural input from TEM and STM images (Fig. 3(b)). In linking theory to experiment we aim to develop greater accuracy simulations by direct comparison of our model output (for example, density of states and transport calculations) with STM tunnelling current results, as well as experimental transport measurements. Such comparisons will enable us to parameterise our TB model directly against experiment rather than to *ab initio* results, as well as provide a means to easily include realistic structural features (defects, strain, vacancies, etc) and system sizes. During this talk I will demonstrate the use of the GRUI and highlight its potential to facilitate the development of greater accuracy models, therefore enabling our physical understanding of nanoscale graphene.

References

[1] Hancock, Y. *et al.*, Physical Review B **81** (2010) 245402.

[2] Huang, B. *et al.*, Physical Review B **77** (2008) 153411.

[3] Girit, Ç.Ö., *et al.*, Science **323** (2009) 1705.

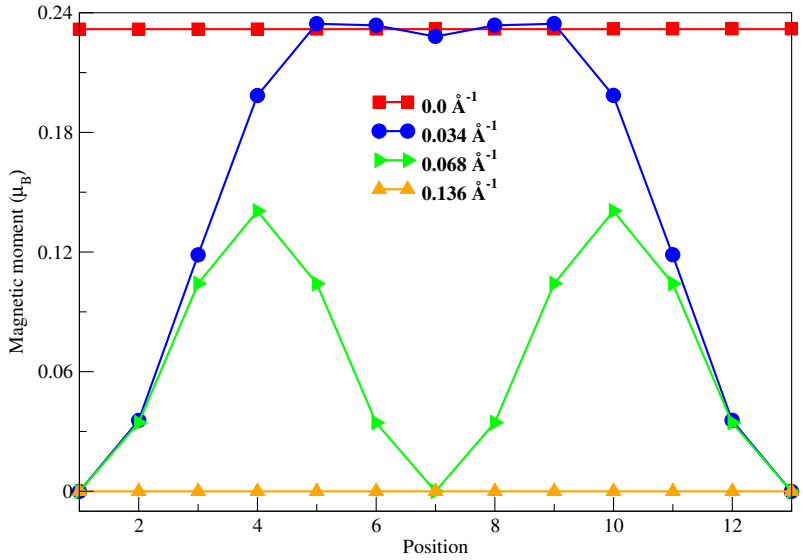


Fig. 1: The generalised TB model is comprised of up to third nearest-neighbor hopping and a mean-field Hubbard-U term. The graph shows the calculated magnetic moment per edge-atom that has been obtained using this model at three systematic edge-vacancy concentrations corresponding to the structures shown in Fig. 2. Comparison with Fig. 1(g) of Ref [2] demonstrates the high-level of accuracy of the TB model against ab initio calculations.

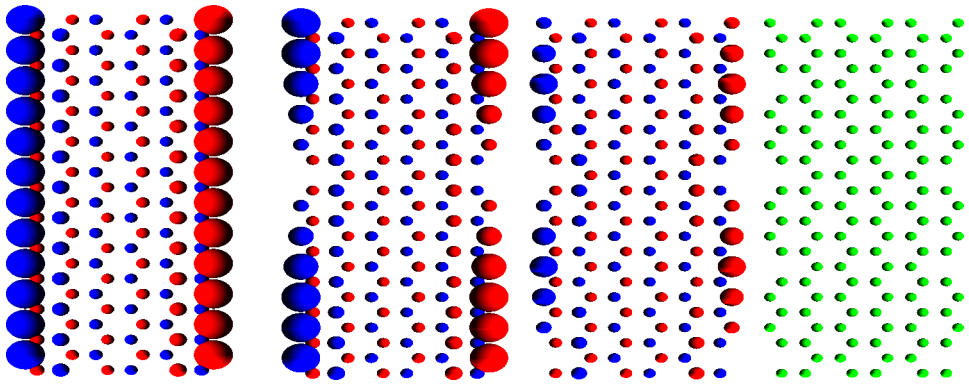
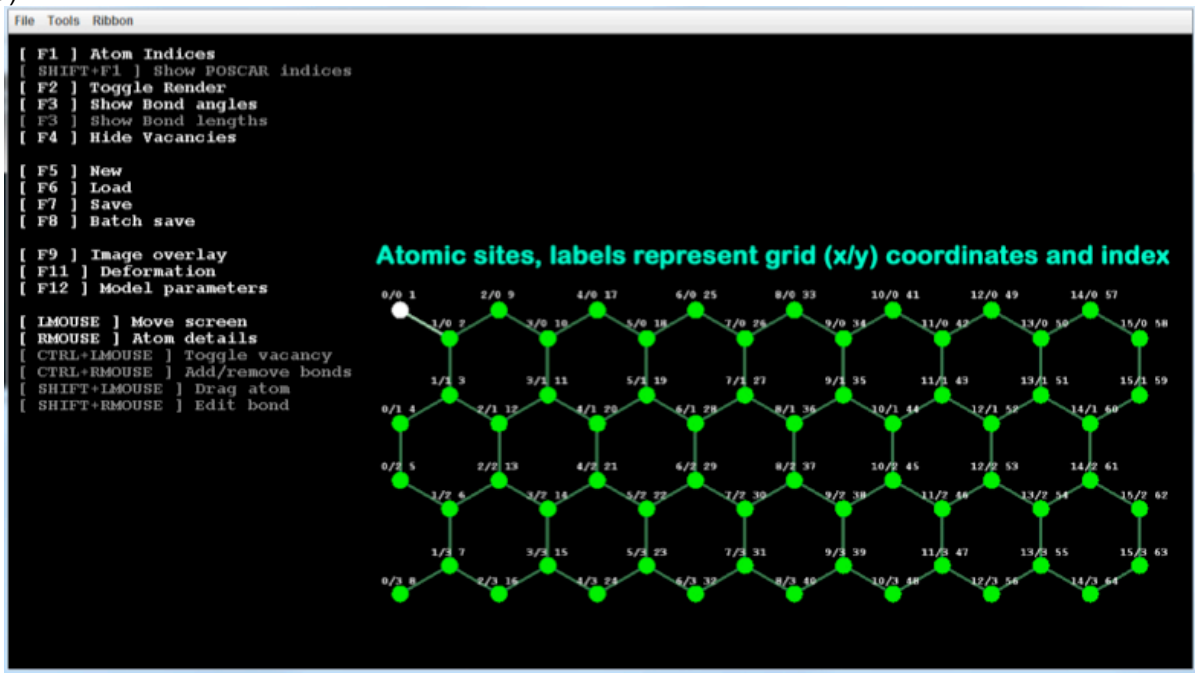


Fig 2: Zig-zag nanoribbon structures showing the computed local net spin-polarisations as obtained from the generalisd TB model. Here red (blue) refer to a net spin-up (spin-down) and green refers to a zero local spin-polarisation. The structures correspond to the calculated local magnetic moment per atom (Fig. 1) and from left to right are for 0.0Å^{-1}, 0.034Å^{-1}, 0.068Å^{-1} and 0.136Å^{-1} symmetric defected systems, respectively.

(a)



(b)

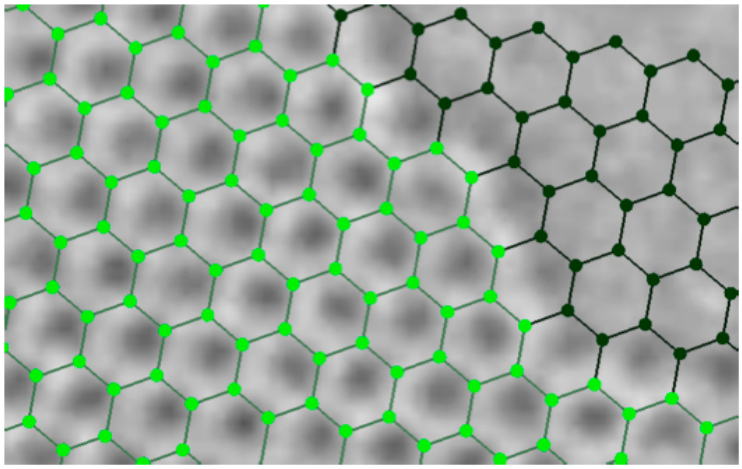


*Fig 3: (a) Screen-shot of the graphic user interface for graphene systems (GRUI) and (b) use of the GRUI showing the overlay of the graphene-mesh onto the experimental TEM result of Girit et al. [3]. The mesh can be positioned over the experimental images and the individual mesh-atoms can be moved so that they sit directly over the experimental result. The GRUI then automatically re-parameterises the TB model to take into account the local atomic perturbations. Experimental image from Girit, Ç.Ö., et al., Science **323** (2009) 1705. Reprinted with permission from AAAS.*