Investigating the electronic and magnetic properties of disordered graphene systems with machine-learning

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Graphene and other 2D materials are very appealing for nanoelectronics, since they could play crucial roles in future nanodevices. At the nanoscopic scale, geometrical effects can critically affect electronic, magnetic, and transport properties. For example, zigzag-edged graphene nanoribbons (ZGNRs) can display spin-polarized edge states, which have very promising applications in future spintronics[1,2]. However, disorder in the lattice structure, derived from either defects or external impurities, is extremely difficult to completely eliminate, and can lead to substantial changes in the properties of these systems. Therefore, characterising the effects of realistic disorders on device behaviour remains crucially important.

Theoretical predictions of large-scale disordered systems can be costly, considering the computational resources required to deal with increases with system size. Machine learning techniques have been employed in various fields, such as consumer recommendation systems, aeronautics and chemistry[3], to exploit patterns in data and make predictions. In this work, we employ machine learning techniques to estimate the properties of two particular disordered graphene systems, and compare their performance against conventional techniques.

Following [4], we first consider electronic transport through a disordered nanoribbon, and show that both kernel ridge regression and neural network techniques can be used to accurately estimate transmission profiles. Secondly, we demonstrate that the magnetic moments of finite graphene flakes, usually calculated using a time-consuming self-consistent procedure, can be predicted using neural networks. In both cases, a careful choice of descriptor greatly improves the performance of the machine learning techniques. Our results highlight the ability of machine learning techniques to capture the complexity of disordered nanostructures, and suggest that they can be used to complement conventional techniques to better understand a wider array of systems.

References

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Figures

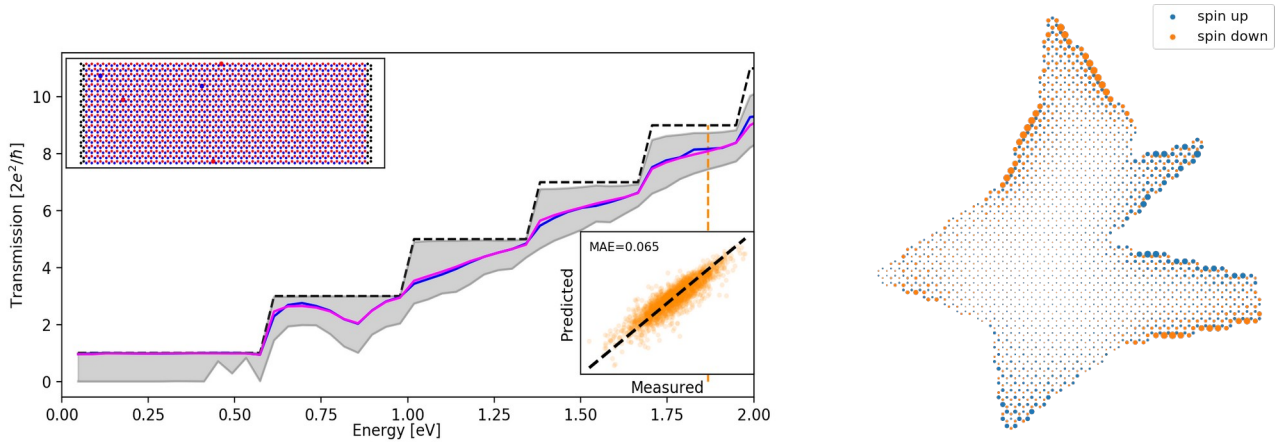

Figure 1: (Left): Actual (purple curve) vs. predicted (blue curve) transmissions for a random disordered ZGNR configuration represented in the upper-left inset with sublattice polarised (red/blue points) impurities. The grey background corresponds to the extremal values of randomly-generated configurations to train the ML model. The lower-right inset refers to the predicted vs. measured transmission for a particular energy.
(Right): Magnetic moment profile of a randomly-generated graphene flake computed with a neural-network.