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Charge, Thermal and Spin Transport in Graphene Composites & Polycrystalline Heterostructures

Abstract

I will discuss charge, thermal and spin transport in chemically and structurally complex forms of graphene accounting from substrate effects, polycrystalline morphology of CVD graphene (and hBN), and chemically functionalization; all aspects being of crucial relevance for the development of applications in flexible and transparent electronics, energy harvesting and spintronics. Multiscale simulation and predictive modelling will be shown to enable simulations of physical properties in realistic models of very large system sizes (with up to 1 billion atoms), reaching the experimental and technology scales.

After introducing some challenges about the modelling of graphene composites I will present quantitative analysis of charge and thermal transport properties in graphene materials in presence of structural imperfections as produced during the wafer-scale production of graphene through chemical growth (CVD), the chemical transfer to versatile substrates, and the device fabrication. Fundamental properties of charge mobilities in polycrystalline graphene, accounting the variability in average grain sizes and chemical reactivity of grain boundaries as observed in real samples grown by CVD will be presented, together with their relevance for device optimisation and diversification of applied functionalities such as chemical sensing [1].

In a second part, I will also briefly explain the current state-of-the-art in understanding spin transport in graphene and how spin manipulation can be engineered through the fabrication of van der Waals heterostructures, fostering progress towards the design of non-charge based revolutionary information processing and computing

References

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