Fundamentals of Charge Transport in Polycrystalline graphene and hybrids

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Abstract

In this talk, I will discuss charge transport in complex forms of graphene (chemically reduced, polycrystalline graphene, chemically functionalized) of relevance for current and future applications in flexible electronics, energy harvesting and spintronics. The crucial contribution of multiscale simulation will be illustrated, demonstrating an achieved high level of predictive capability for very large system sizes (with up to 1 billion atoms), reaching the experimental and technology scales.

The main illustration will be the quantitative analysis on the transport properties of structural imperfections produced during the wafer-scale production of graphene through chemical growth (CVD), or the mechanical/chemical exfoliation and chemical transfer to versatile substrates, followed by 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 optimization and diversification of applied functionalities such as chemical sensing.

References

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