Students' Annual Seminar

Finite Size Effects in Graphene Oxide Models

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Oxidation of graphene followed by exfoliation of the graphene layers generates graphene oxide (GO). GO has gathered a lot of attention over the last decade due to its impressive mechanical and electronic properties, e.g. large surface area, hydrophilicity, chemical reactivity and its ability to easily integrate with other materials through surface functional groups. GO possesses defects of various kinds. Percentage of non-graphitic carbon is usually taken as the metric to quantify the amount of the defects present. In this talk, I will show that while this metric is fine at very large defect concentrations, it fails to properly identify the amount of defects when the defect density is low. In this study I will introduce a new parameter that can track the defects in both the regimes. Furthermore, I will show that the defect distribution is quite sensitive towards the size of the simulation cell whereas the stress-strain response seems to be more robust. Moreover, I will discuss how the new metric tracks the structural response under shear.

Friday, Mar 31st 2023

5:00 PM

CR-1, TIFR-H