Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Students' Annual Seminar

Role of defects in modulating Young's modulus and Raman response of graphene oxide: a computational exploration

Sownyak Mondal

Graphene oxide (GO) exhibits versatile properties that are modulated by defects. Molecular dynamics simulations with ReaxFF force field parameters have been successfully employed to generate realistic GO structures with different kind of defects by varying Oxygen (O)/Carbon (C) ratio. We introduce here a hitherto unexplored metric, relative minimum area, to quantify defects. This novel metric is shown to be more sensitive towards structural roughness albeit being exclusive to the defects as compared to the traditional way of estimating defect density. We also investigate the role of defects in modulating Young's modulus and uncover strategies to fine tune the modulus with point substitutions. The extent of defects in graphitic materials is often characterised by measuring the ratio of intensities of the characteristic peaks for defect (D) and graphitic (G) regions in Raman spectra. However, this ratio is non-monotonic with respect to defect density. Employing machine learning techniques, we analyse the normal modes to decipher the origin of this non-monotonic behaviour.

Wednesday, Mar 27th 2024

14:00 Hrs (Tea / Coffee 13:45 Hrs)

CR-4, TIFR-H