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Effect of Hydroxyl Functionalization on the Mechanical and Fracture Behaviour of Monolayer Graphene

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Abstract : The aim of this article is to study the effects of hydroxyl functional group on the mechanical strength and fracture toughness of graphene. This functional group forms the backbone of intrinsic atomic structure of graphene oxide (GO). Molecular dynamics-based simulations were performed in conjunction with reactive force field (ReaxFF) parameters to capture the mode-I fracture toughness of hydroxyl functionalised graphene. Moreover, these simulations helped in concluding that spatial distribution and concentration of hydroxyl functional group significantly affects the fracture morphology of graphene nanosheet. In contrast to literature investigations, atomistic simulations predicted a transition in the failure morphology of hydroxyl functionalised graphene from brittle to ductile as a function of its spatial distribution on graphene sheet.

Keywords : graphene, graphene oxide, ReaxFF, molecular dynamics
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