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**Computational Investigation of Graphene-Carbon Nanotube-Polymer Composite** SANJIV JHA, MICHAEL ROTH, GUIDO TODDE, GOPINATH SUBRAMANIAN, Univ of Southern Mississippi, MANOJ SHUKLA, US Army Engineer Research and Development Center 3909 Halls Ferry Road Vicksburg, MS 39180, USA, UNIV OF SOUTHERN MISSISSIPPI COLLABORATION, US ARMY ENGINEER RESEARCH AND DEVELOPMENT CENTER 3909 HALLS FERRY ROAD VICKSBURG, MS 39180, USA COLLABORATION — Graphene is a single atom thick two dimensional carbon sheet where $sp^2$-hybridized carbon atoms are arranged in a honeycomb structure. The functionalization of graphene and carbon nanotubes (CNTs) with polymer is a route for developing high performance nanocomposite materials. We study the interfacial interactions among graphene, CNT, and Nylon 6 polymer using computational methods based on density functional theory (DFT) and empirical force-field. Our DFT calculations are carried out using Quantum-ESPRESSO electronic structure code with van der Waals functional (vdW-DF2), whereas the empirical calculations are performed using LAMMPS with the COMPASS force-field. Our results demonstrated that the interactions between (8,8) CNT and graphene, and between CNT/graphene and Nylon 6 consist mostly of van der Waals type. The computed Young's moduli indicated that the mechanical properties of carbon nanostructures are enhanced by their interactions with polymer. The presence of Stone-Wales (SW) defects lowered the Young's moduli of carbon nanostructures.

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