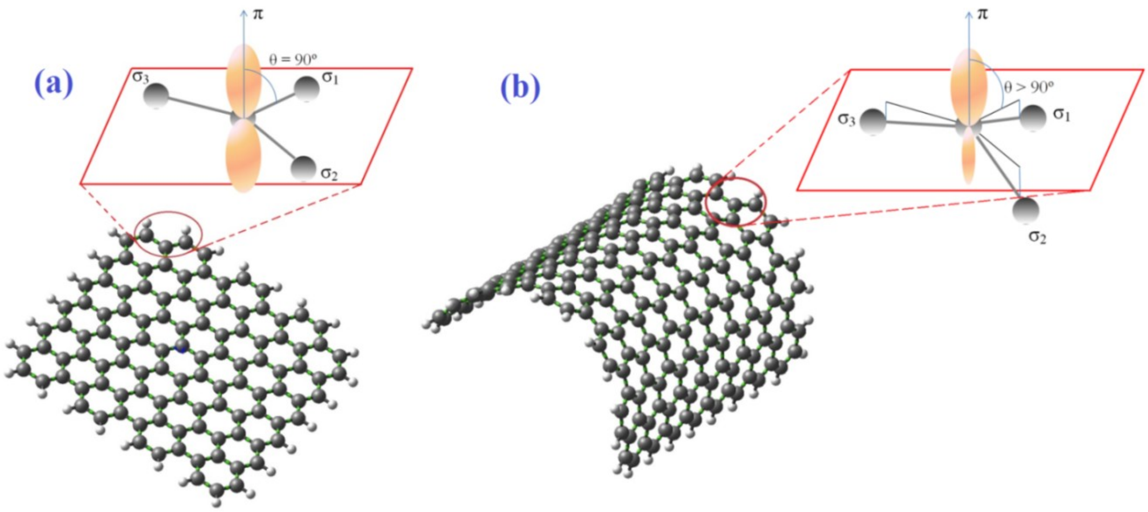
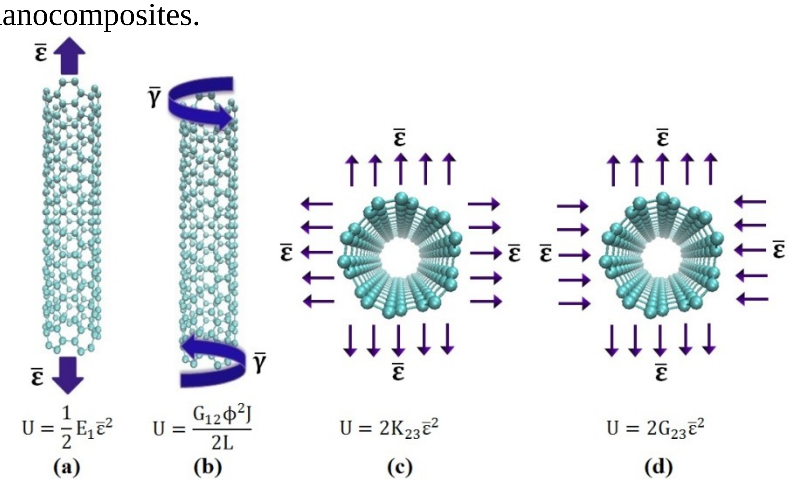
Flexoelectricity in 2D Nanomaterials: Flexoelectricity phenomenon is the response of electric polarization to an applied strain gradient and is developed as a consequence of crystal symmetry in all materials. Symmetry breaking at surfaces and interfaces and the capability to undergo large strain gradients in nanoscale systems induces unusual forms of electromechanical coupling due to flexoelectricity phenomena. The recent study by Dr. Kundalwal showed that the presence of strain gradient in non-piezoelectric graphene sheet does not only affect the ionic positions, but also the asymmetric redistribution of the electron density, which induce strong polarization in the graphene sheet. Using quantum mechanics calculations, the resulting axial and normal piezoelectric coefficients of the graphene sheet were determined using two loading conditions: (i) a graphene sheet containing noncentrosymmetric pores subjected to an axial load, and (ii) a pristine graphene sheet subjected to a bending moment. This fundamental study highlights the possibility of using non-piezoelectric 2D nano layers sheets in nanoelectromechanical systems as sensors or actuators.



Graphene systems in which π-orbitals are (a) symmetric, and (b) asymmetric [*Carbon*, **117**, 462-472 (2017)]

Molecular Dynamics (MD) Simulations: MD simulations were conducted to determine the transversely isotropic elastic properties of carbon nanotubes containing vacancies. This is achieved by imposing axial extension, twist, in-plane biaxial tension and in-plane shear to the defective CNTs, as shown below. This fundamental study highlights the important role played by vacancy defected CNTs in determining their mechanical behaviors as reinforcements in multifunctional nanocomposites.



Four types of loading conditions: (a) tensile, (b) twist, (c) in-plane bi-axial tension, and (d) in-plane shear [*Acta Mechanica* (2018), doi: 10.1007/s00707-018-2123-5]