Strain mediated nanoscale transport in nanostructured carbon materials
Hossain, Md, zubaer@caltech.edu, California Institute of Technology

ABSTRACT
Low-dimensional materials such as graphene or carbon nanotube show remarkable promise for next generation electronics (transistors), structural materials (composites), energy (thermoelectrics, solar cells), and biology (biosensors, drug delivery). However, owing to nanoscale dimension they are very susceptible to undergo mechanical deformation and respond to electronic interactions. As a result, their pristine properties are altered substantially in the vicinity of insulating substrates (on which they are grown), electrodes (that they are attached to) as well as external reactive molecules such as H₂O. To quantify how deformation affects transport across the interface and how it couples with nanoscale deformation, this research uses DFT simulations and studies the coupling between deformation and electronic properties in graphene–SiO₂ and CNT–SiO₂ heterointerfaces. It is found that the type of surface passivation and interacting site play a critical role in modulating the interfacial transport mechanisms. In addition, to quantify the effect of local strain on quantum conductance in graphene, we explore the implication of hydrostatic or uniaxial deformation on electrons surrounding the Fermi energy. Although hydrostatic deformation preserves the symmetry of band deformation and influences quantum conductance in a symmetric manner, uniaxial strain modulates quantum conductance asymmetrically with respect to the Fermi energy. Subsequently, amount of conductance alteration is different for the holes and electrons. For either type deformation, strain substantially modifies conductance and highlights the importance of exploring the role of mechanics in controlling or altering fundamental properties in nanostructured materials. The study provides important mechanical signatures for controlling transport properties in low-dimensional materials.