**Characterization of nano carbon at material interfaces**

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Carbon nanotube (CNT) and graphene have attracted major interests due to their exceptional electrical, mechanical, and thermal properties. CNT/graphene based nanocomposites can be applied to flexible display, photovoltaic cell, and electromagnetic-wave interference materials. Carbon nanotube (CNT) and graphene have been also applied to energy storage devices such as batteries and supercapacitors. As active materials or key components in electrodes, they play an important role in improvement of energy or power densities and structure stability. In spite of these promising applications, fundamental understanding of the phenomena at nano carbon/ matrix interfaces is still lacking. To this, we have systematically investigated the mechanical, thermal and electrical properties at CNT/graphene polymer interfaces for applications in nanocomposites and energy storage devices.

We find that the strength of graphene is sensitive to atomic defects. Oxygen-functionalized graphene leads to increased interface adhesion between graphene and polymers, as compared to hydrogen-functionalized and pristine graphene. Therefore, graphene oxide can be used to reinforce polymer nanocomposites. Graphene layer can enhance the yield strength of metallic substrates, confirmed by our experimental and numerical studies. Grafting polymer chains on top of graphene can significantly improve the graphene/polymer interface thermal conductivity, due to reduced thermal mismatch. The electrical conductivity of CNT/graphene polymer composites can be predicted using numerical approaches, leading to the development of flexible strain sensors. For energy storage applications, we have investigated the effects of structure and heteroatom doping on the interfacial interactions between graphene and other active materials in batteries. In Li-S batteries, we find porous graphene with oxygen functional groups is an effective cathode material, attributed to the Li-O covalent bonds retaining polysulfides and improving electrode conductivity. In Na-ion batteries, our modeling indicates that heteroatom doped-graphene is a potential anode material. Graphene doped with pyridinic-N, pyrrolic-N, F and B improves the electrochemical Na storage due to increased electron deficient sites. On the other hand, P doping improves the Na storage ability due to the geometric effect caused by bond length mismatch. In contrast, the introduction of graphitic-N and S into graphene is inefficient for Na storage because of their inability to accept electrons from Na.