

Some studies on pristine and functionalized graphene using first principles calculations

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In this talk, I like to present some of recent work carried out on pristine and functionalized graphene using first principles study. The first part of my talk will be on tuning the electronic property of graphene [1] and the second half will be on investigation of hydrogen storage on strained graphene [2]. All the calculations are carried out using VASP. The emergence of band gap in this semimetal can be accomplished through different mechanisms. The band gap modulations in graphene through chemical functionalization with oxygen and through the creation of vacancies (Fig. 1) have been reported. The covalent functionalization with oxygen results in the structural and band gap modifications that depend on the adatom (oxygen) coverage. The curvature induced in graphene under full coverage case suggests the folding of the graphene sheets through functionalization. This is the new epoxide structure. The vacant site in graphene should be the preferential site for adsorption of foreign chemical species, because it has rich charge and distorted carbon environment. All these above mechanisms alter either electronic properties or both structural and electronic properties of graphene. As a result, these mechanisms completely destroy the nature of massless Dirac fermions of graphene. Also, the effect of static electric field on the band gap in hydrogenated graphene (graphane) is studied. The combined action of structural modifications that involves stretching and compression of C–C bonds in the hexagonal network and charge transfer mechanism are responsible for the gap opening in electronic spectrum of graphene, which is essential for the near future application of graphene in electronics.

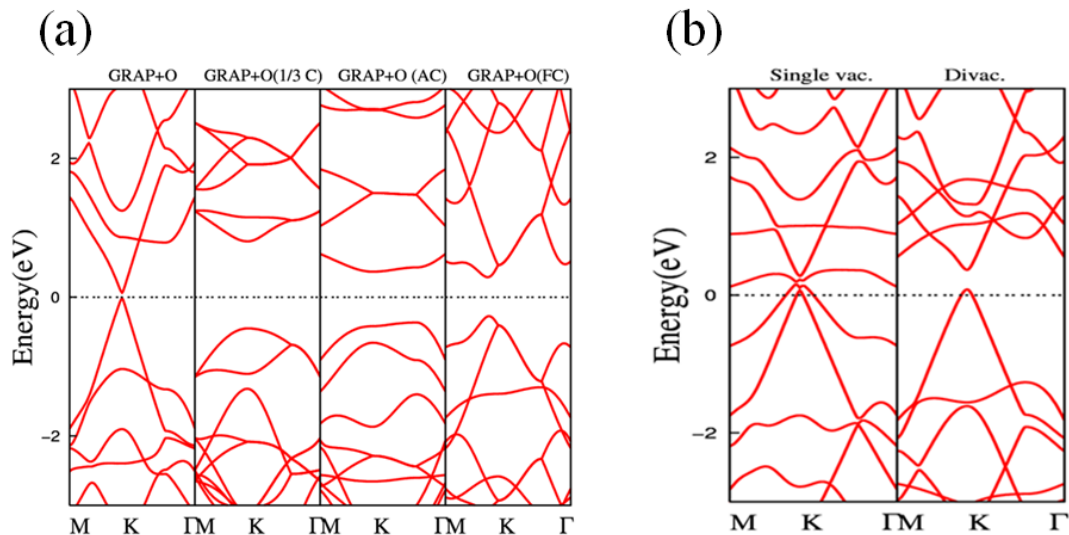


Figure 1 - Band Structure of graphene with (a) different coverage of oxygen and (b) mono and divacant sites.

Also, it is shown that chemically inert monolayer graphene becomes active by strain engineering. The sheets are stretched biaxially to introduce strain of 1.43%, 5%, 8.5% and 10% in the C–C bond lengths. The introduction of strain enhances the chemical reactivity of graphene surface and hence they become chemically more active than the pristine one. Under strained environment the carbon atoms are enriched with quasi-localized p electron clouds (Fig. 2) and the uneven distribution of charges is responsible for the binding of borane and hydrogen molecules on graphene. Thus this study highlights the interplay between the induced strain and adsorption of chemical species. The interaction of molecular hydrogen increases with increase in strain in the substrate (strained graphene). Since graphene sheets can be freely suspended without any substrate, we can stretch the sheets by tuning distance between the clamped edges of the holding frame. In this way, stacks of stretched graphene sheets can be manufactured and a good hydrogen storage medium can be obtained. Overall, this study underlines that the introduction of strain is a non-destructive technique and the chemical properties of graphene can be manipulated through strain engineering that unlocks the doors for a new electronic, optical and hydrogen storage device technologies.

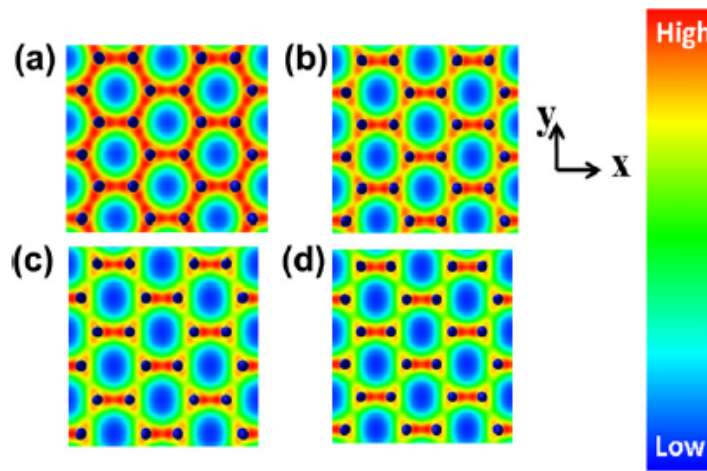


Figure 2 - Charge profile of biaxially SG (a) 1.43%, (b) 5%, (c) 8.5% and (d) 10%.

Thus, suitable mechanism can be adopted to get desirable property using graphene to fulfill necessary applications.

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References:

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2. V. J. Surya, K. Iyakutti, H. Mizuseki and Y. Kawazoe, Modification of graphene as active hydrogen storage medium by strain engineering, *Comp. Mat. Sci.*, 65, 144–148, 2012.