WHY DO WE NEED HETEROATOMS FOR ACTIVATING CARBON FOR HYDROGEN STORAGE APPLICATIONS

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In this presentation we wish to list some relevant points on the topic above:

1. **Carbon surface by itself is in capable of activating molecular hydrogen possibly due to its predominant covalent character.**
2. **The presence of heteroatoms in carbon framework possibly exposes more of Lewis acid or base sites which are possibl the active centres for the generation of atomic hydrogen.**
3. **C-C bond distance typicaly varies between 120 to 154 pm in carbon materials and thei may not be suitbale for molecular hdyrogen activation since the bond distance in hydrogen is only 74 pm.**
4. **The question is why covalent systems like carbon materials do not activate hydrogen molecule while hetero atoms possibly do? One argument that was proposed in the previous point is from the geometry based. Possibly also the dissociation of hydrogen molecule is an activated process and population of its antibonding molecular orbital may be necessary to effect dissociation and this is possibly achieved without prior dissociation of hydrogen and this population of electron density in the antibonding state is possible by the lone pairs of electrons available in hetero atoms.**
5. **Possibly the energy states of carbon system are not energetically not appropriate for populating the antibonding state of molecular hydrogen but the nonbonding states of hetero atoms may be of similar energy.**
6. **It has been already argued by us in terms of redox potential and as well as in terms of free energy variation that heteroatoms are possibly the activating centres for hydrogen molecule. The validity of these arguments can be seen elsewhere.**
7. **The geometrical arrangment of boron atoms at alternate positins has been postulated by us as possible active sites for hydrogen activation.**
8. **Since rthe activated hydrogen atoms have to migrate to carbon lattice the activating centres should not bind the hydrogen atoms strongly. This may be the case wit heteroatoms while metals may hold the hydrogen atoms strongly in one of the three bonding states and hence may not facilitate the cross over of hydrogen to the carbon lattice.**
9. **It has been postulated that hydrogen activation has to be in the form of hydrogen atoms and not in any other form like proton or hydride ion, and this will take place if the geometry of the adsorption sites are suitable (which is possible in metallic lattice) for homonuclear bond breakage, but the strong binding makes the migration difficulty. However the charge sharing which is possible in the case of heteroatoms may possibly facilitate the homonuclear fission of the hydrogen-hydrogen bond and the charge populating the antibonding orbital of hydrogen molecule finally ending up as lone pair electrons in the heteroatom. The time scales of this charge population and also the bond breakage and migration may be matching**

so that this process takes place on heteroatom substituted carbon materials. However we have to make more in depth analysis and hope this will be possible in the near future