

## **Seminar**

### **Mapping the Hydrogen Evolution Reaction in Graphene-hBN van der Waals Heterostructures**

**Sumit Bawari**

**TCIS, Hyderabad**

Advances in van der Waals (vdW) heterostructures of atomic layers open up the possibility of new vertical quantum hetero-junctions with atomically sharp interfaces. Recent research on viable energy resources opens up possibilities of hydrogen as a promising energy source, where electrochemical hydrogen evolution reaction (HER) is a carbon neutral method to obtain pure hydrogen. In this work, we study the possibilities of graphene (G) and hexagonal boron nitride (hBN) based vertical heterostructures as heterogeneous catalysts for HER. Covalently bonded in-plane doped graphene systems have previously been researched where; in-plane covalently bonded h-BN with graphene shows unusual photo and electro catalytic HER activities. Experimentally, we find that vdW heterostructures of G/hBN and hBN/G exhibit enhanced HER activity, with stacking dependant behaviour. This enhanced activity is studied through Molecular dynamics (MD) simulations and Density Functional Theory (DFT) calculations that provide insight into the sorption behaviour and charge transfer efficiency respectively, for efficient catalysis. Using both methods, we discover catalytically active sites on the G/hBN interface and try to justify the experimental observations.

***Monday, Oct 8<sup>th</sup> 2018***

***11:30 AM (Tea/Coffee at 11:00 AM)***

***Auditorium, TIFR-H***