Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Students' Annual Seminar

Role of molecular interfaces and dopants in heterogeneous catalysis

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Our recent studies have shown that graphene-hBN van der Waals vertical interfaces can bring electro-catalytic activities to hybrids though individual layers are not active. The hydrogen evolution activity of these interfaces, mapped using density functional theory analyses and molecular dynamics based simulation studies, prove that the van der Waals shadow effect of hBN makes graphene active towards hydrogen evolution while forming a heterostructure. Previous studies have shown that exciton formation can occur at the graphene-hBN interface, and dipoles formed at the interfaces of graphene-hBN can be long lived to a few picoseconds. We have explored the possibilities of these photo-generated excitons for hydrogen generation and it is shown both theoretically and experimentally that graphene-hBN interfaces can be used for photo-electrocatalytic hydrogen generation. We further show that along with the enhancement in inherent activity of the atomic layer, further enhancement can occur _via_ nanostructuring of these hybrid layers. Apart from molecular interface based catalysts, boron or nitrogen or boron nitride in-plane doped graphene catalysts were also computationally studied for catalysis. Here, we try to bring a principle component analysis approach to identifying the role of different parameters in catalysis. Initial results of this analysis will be discussed during the talk. Also, near future plan on the molecular junctions based transport studies will also be briefly discussed.

Friday, Mar 1st 2019

10:30 AM (Tea/Coffee at 9:45 AM)

Seminar Hall, TIFR-H