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

Students' Annual Seminar

Studies on the Molecular Junctions of Carbon

Shubhadeep Pal

In one of our recent studies[1,2,3], coupling CNTs via a benzene molecule is found to be aiding to the formation of macro/mesoporous CNT sponges and these hybrid structures have augmented hydrogen evolution reaction (HER) performance in comparison to their pristine ones.[1] This enhanced HER activity is found to be emanating from the energy band structure modification after coupling the tubes via a benzene molecule. My studies during the last six months are focussed on the experimental realization of such band structure modification while coupling using scanning tunnelling microscopy/spectroscopy (STM/S). This band modification at molecular junction shows no electronic transmission while in CNT there is high transmission and makes it possible for futuristic molecular switch device. Electrical transport calculations using non-equilibrium Green's function formalism with density functional theory (NEGF-DFT) have been conducted on these junctions to unravel the transport behaviour of these junctions along with the pristine CNT. The initial results along with the future plans on these works will be discussed during the talk.

References:

[1] Covalently Connected Carbon Nanotubes as Electrocatalysts for Hydrogen Evolution Reaction through Band Engineering, **Shubhadeep Pal et. al. ACS Catalysis** 7, 2676-2684 (**2017**).
[2] Hydrogen Evolution Reaction Activity of Graphene-MoS2 van der Waals Heterostructures, ACS Energy Letters, DOI:10.1021/acsenergylett.7b00349 (2017).
[3] Temperature Assisted Shear Exfoliation of Layered Crystals for the Large Scale Synthesis of Catalytically Active Luminescent Quantum Dots, **Shubhadeep Pal et. al. Materials Chemistry Frontiers** 1, 319-325 (**2017**).

Monday, Jan 22nd 2018

03:00 PM (Tea/Coffee at 02:30 PM)

Seminar Hall, TIFR-H