



## Substrate induced modulation of physical and chemical properties of quasi two-dimensional nanostructures

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Indian Association for the Cultivation of Science,  
Kolkata, INDIA
- 日程** : 12月22日(木) 14:00-15:00
- 場所** : 本館1階 H155B 理学院セミナー室

### 概要

In the post-Graphene era, several quasi two-dimensional nanostructures have been grown epitaxially on metallic or semiconducting substrates, resulting in heterojunctions with interesting application potential. Physical and chemical properties of such overlayers often get modulated by the sub-surface layers of the corresponding substrates, leading to manifestation of new properties. In this talk, I shall discuss how density functional theory (DFT) based first principles approach can be used for a microscopic understanding of these interface induced effects. Such phenomena depend crucially on the exact geometry of the interface, which in turn is self-consistently inter-twinned with its electronic structure. I shall illustrate this with some case studies on applications ranging from catalysts for CO oxidation to modulation of electronic properties in devices [1-4].

1. A. Bhattacharya *et al*, Appl. Phys. Lett. **103**, 123113 (2013).
2. A.H.M. Abdul Wasey *et al*, ACS Appl. Mater. Interfaces **5**, 10404 (2013).
3. A.H.M. Abdul Wasey *et al*, AIP Advances **4**, 047107 (2014).
4. P. Banerjee *et al*, Appl. Surf. Sci. (2016), in press.

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