Tata Institute of Fundamental Research
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Seminar

Functional Materials Approaching Molecular Scale: Insights from Electron Microscopy, Simulations & Designed Experiments

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For quite some time now, breakdown of conventional wisdom at the atomic scale has greatly facilitated the exploration of the 'room at the bottom.' In this quest, atomic-scale electron microscopy has played a significant role, sometimes even leading to discovery of new structures (e.g. carbon nanotube) under electron microscope. Likewise, many computation-intensive atomistic simulations have come up with predictions which can be verified through electron microscopy, along with design of new experiments. In this talk, I will focus on some of such guided microscopy, and designed experiments for different nanomaterials.

The first part of the talk will consist of the structural aspect of ultrathin Au nanowires, wherein the {111} atomic planes of these nanowires undergo wrinkling, leading to formation of saddle surfaces. This has been captured in our simulations, followed by experimental verification through aberration-corrected transmission electron microscopy. Very recent scanning transmission electron microscopy experiments with similar scale Pt nanowires show that with a priori crystallographic information, it is possible to reconstruct a 3-D structure from a single projection image of the material. Furthermore, I will discuss the significant difference of electronic structure of the Au nanowires from bulk Au, which has been predicted in simulations, and later verified in experiments.

The second part will address the electronic properties of ultralow band gap Te nanowires, where the electronic structure of the wire can be engineered with analyte adsorption. Once again, simulations with simple adsorption of NO_2 on these nanowires show a semiconductor to metal transition, which was verified by experiments and low-temperature R-T measurements.

In the third and last part, I will focus on the synthesis of the electrochromic tungsten oxide. The strategically synthesized phases, namely hexagonal and orthorhombic WO_3, exhibit very different electrochromic switching and diffusion behavior upon proton intercalation. Phase selection, growth mechanism and electrochromic behavior – all can be explained through computed electronic interactions.

Thursday, Aug 16th 2018

4:00 PM (Tea/Coffee at 03:30 PM)

Auditorium, TIFR-H