

## Colloquium

## Functional Materials at Atomic Limit: Synergistic Investigations through Electron Microscopy & Simulations

## **Ahin Roy**

## IISc, Bangalore

Atomic resolution electron microscopy and atomistic simulations can play a synergistic role to understand structure-property relationship in functional nanomaterials. This talk will focus on some of such cases involving different nanowires and oxide materials.

The first part of the talk will consist of the structural aspect of ultrathin metal nanowires, wherein using aberration-corrected transmission electron microscopy (TEM) or scanning transmission electron microscopy (STEM), we can interrogate their structure at atomic scale, often corroborating with simulations. The second part will deal with the electronic properties of ultrathin Te nanowires, wherein we see an adsorption-induced semiconductor to metal (S-M) transition in simulations, further verified by experiments. In the third and last part, I will focus on the synthesis of the phase dependent electrochromic behaviour of tungsten oxide. The strategically synthesized phases, namely hexagonal and orthorhombic WO<sub>3</sub>, 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.

Wednesday, Nov 28<sup>th</sup> 2018 11:30 AM (Tea/Coffee at 11:00 AM) Auditorium, TIFR-H