Title:

Application of '*Ab Initio* quantum mechanical computations' for nanomaterial characterisation for photovoltaic/solar Energy Applications

By

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ABSTRACT

Over past few decades much of energy research is focussed on renewable energy sources including solar energy through light energy harvesting through a medium (generally a semiconductor) conversion to electricity, clean fuel generation (such as water splitting), Dye sensitised and perovskite solar cells etc. are categorised as emerging solar energy technologies. The material characteristics are obviously the key factors for selecting the best options for various technologies. This characterisation could be possible through various fundamental and advanced experimental spectroscopic methods. The advanced experimental methods could sometimes consume money and time. Computational predictions of material characteristics, could be helpful in deciding whether to pursue experimental procedures or not.

In this talk the fundamental concept of the *Ab Initio* Density Functional Theory (DFT) based material characterisation is introduced and few case studies are discussed while predicting electronic band structures, Phonon spectrum, Ab Initio Molecular dynamics (AIMD) etc. The focus is on Two-dimensional (2D) nanomaterials for predicting the properties for various photovoltaic applications.

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