The 201st MANA Special Seminar

First Principles Modelling for Dye-Sensitised Solar Cells

Chair: Dr. Masakazu Aono (MANA Director-General)

Prof. David Bowler

(Department of Physics & Astronomy, University College London, UK)

I will describe the recent computational work in the Cambridge MANA Satellite at UCL on the fundamental processes in dye-sensitised solar cells (DSSCs). By understanding the basic science of DSSCs, we can improve their design and efficiency. I will consider the atomic and electronic structure of particular dyes on TiO2, the early stages of growth of thin alumina layers on TiO2, and recent computational advances (linear scaling DFT, constrained DFT and time-dependent DFT) which will allow accurate modelling of electron transfer processes from the dye to the substrate.

Venue: **Seminar Room #431, MANA Bldg.**

Date: **April 7th (Thursday)** ***Time:*** **15:30-16:15**

NAMIKI Site

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