Application for class B usage of ICHEC facilities

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Abstract

The search for materials for a new generation of solar cells has inspired a great deal of work on dye-sensitized solar cells (DSSCs). DSSCs consist of a wide-bandgap semiconductor (usually, a metal oxide such as TiO_2 or ZnO) that is sensitized by an organic dye. The addition of dyes onto the metal oxide surface enhances the photoactivity of the oxide as compared to the pure semiconducting state. Although a few prototypes of such cells have been successfully fabricated by several groups worldwide, the efficiency of these cells is much lower than their silicon counterpart. In addition, there is no clear consensus on the mechanism(s) behind one of the key steps involved in the function of DSSCs: charge injection from the dye molecule into the metal-oxide. This is primarily due to two reasons: the field, at present, lacks a clear picture at the quantum mechanical level and there are several injection mechanisms that can come into play either exclusively or together, affecting the efficiency of the cells. The aim of this research is to address several of the issues at the quantum mechanical level. The work will be carried out using state-of-the-art density functional theory (DFT) calculations as well as newer developments in this field that take the calculations at a level beyond DFT. Ultimately, we hope to provide a theoretical framework for the selection of the right class of dyes to act as the sensitizers for the metal oxide (here, TiO_2).