
O 94: Invited Talk (Ralph Gebauer)

Time: Friday 10:15–11:00

Location: TRE Phy

Invited Talk

O 94.1 Fri 10:15 TRE Phy

Computational study of optical and structural properties of an organic dye sensitized solar cell — •RALPH GEBAUER¹ and FILIPPO DE ANGELIS² — ¹The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy — ²Istituto CNR di Scienze e Tecnologie Molecolari (ISTM), c/o Dipartimento di Chimica, Università di Perugia, Italy

Dye sensitized solar cells are intensely studied as possible low-cost alternatives to traditional silicon based photovoltaic devices. For further progress in this technology, a detailed understanding of the dye/semiconductor heterointerface and of the interactions of the dye molecules with the surrounding electrolyte is crucial.

In this talk, we will present *ab initio* molecular dynamics simulations of a dye sensitized semiconductor surface immersed in an explicit water environment. This simulation is complemented by time-dependent density functional theory computations of the optical properties of the whole system (surface + dye + solvent). This technique allows us to gain unprecedented insight into the excited states and the dynamics of the solvated system at room temperature.

We are able to reproduce the experimentally observed asymmetry of the absorption spectrum and provide an estimate of the effect of thermal fluctuations on the driving force for electron injection. Finally, we are able to provide a detailed picture of possible dye desorption dynamics in such systems.