



Mercoledì **3 luglio 2019** alle ore **14:30** presso l'aula L1

il Dr. Joshua D. Elliott

School of Chemical Engineering and Analytical Science, University
of Manchester

terrà il seminario dal titolo:

Time-evolution of excitonic states from many-body perturbation theory: Modelling electron injection in dye-sensitized solar cells.

I will present simulations of the chromophore-to-semiconductor electron injection step in a model dye-sensitized solar cell. Excitonic effects are introduced through the solution of the Bethe-Salpeter equation and maintained during the time-evolution steps applying the two-particle Hamiltonian matrix.

The approach is summarized in a three-step computational workflow:

- (i) The BSE is solved for in a subspace of the system relevant to the initial excitation, in this case localized on an adsorbed dye molecule,
- (ii) excitonic states are projected onto the full simulation cell and complete electronic manifold and
- (iii) the electron and hole are dynamically propagated to simulate the injection process.

The calculations provide details on the rate of electron injection, evolution of the exciton binding energy and on the disentanglement of the electron-hole pair.

The method introduced is versatile and can be applied to other instances where electron transfer takes place between strongly coupled states.

La presenza della S. V. sarà molto gradita