First-principles methods based on many-body perturbation theory (MBPT) proved to be the solution to the scarce accuracy of ordinary density functional theory for the evaluation of excitation properties. However, such approaches are much more computational demanding. In the last years we have introduced a scheme for calculating electronic properties with the MBPT GW-BSE approach which is particularly suitable for calculations in large model structures eliminating the major drawback of sums over empty one-particle orbitals. Recently, we have extended our method to the evaluation of optical absorption spectra and of exciton binding energies.

First, I will discuss how we could use our methods for investigating the alignment of energy levels in dye sensitised solar-cells which is at the very base of their functioning. I will show how we could successfully predict energy levels alignment leading to estimations for the maximum attainable open-circuit voltage including solvent effects.

Then, I will present our GW results for the modelling of solar cells based on hybrid organic-inorganic perovskites. In particular, I will show that the correct treatment of spin-orbit coupling is essential for a correct description of the excitation properties such as band gaps.