Large scale GW-BSE calculations with O(N^3) scaling: application to dye sensitised solar cells

A talk by Paolo Umari

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I will present our method which permits to lower the cost a of ordinary first-principles many-body perturbation theory GW-BSE calculations of excitation properties from O(N^4) to O(N^3) scaling with respect to the generic system size N. This is achieved through the representation of the manifold of occupied one-particle orbitals in terms of maximally localised Wannier's functions. Moreover, we avoid any explicit sum over empty one-particle orbitals. The present implementation, as a module of the Quantum-Espresso package, is based on the plane-waves pseudo-potential paradigm.

I will illustrate the potential of our approach presenting the application to a realistic model structure of a dye-sensitised solar cell which we could afford even with only moderate computational resources. Indeed, we found that the GW-BSE approach provide a quantitative picture of interfacial excited state energetics in organic dye-sensitized TiO2 in nice agreement with available experimental figures.

Finally, I will discuss possible future extensions of our method.