Polaronic contribution to band-structures within the GW approximation

To go beyond simple density functional theory (DFT), and to obtain reliable quasi-particle energies, the GW approximation of many-body perturbation theory emerged over the years as an invaluable tool. The GW approximation, introduced in 1965 by Lars Hedin\(^1\), allows one to determine the “true” single-electron addition and removal energies, also called quasi-particle energies. The standard use of this theory, known as perturbative GW, starts from a DFT calculation and evaluates the corrections to the band-structure perturbatively, i.e., ignoring the self-consistent process. It is clear that this procedure is justified when the departure wavefunctions are already close to the quasiparticle ones. This is the case in many systems, like simple sp semiconductors.

However, perturbative GW has proved to be insufficient for interesting systems, including the important class of transition metal oxides. One possible solution is performing (restricted) self-consistent GW\(^2\). This latter method has been applied, e.g., to transparent conductive oxides\(^3\) and to Cu(In,Ga)(S,Se)\(_2\), used in thin-film solar cell technology\(^4\), yielding excellent results for the quasiparticle band-structure.

Self-consistent GW has to a large extent solved the electron-electron correlation problem. However, one should keep in mind that phonons also play a very important role in the quasiparticle and absorption spectrum of polar materials. In fact, polaronic effects can reduce the band-gap by more than 1 eV for materials as common as NaCl\(^5\). Unfortunately, up to now the polaronic contribution has only been included in GW calculations using very simple models\(^5\).

This project proposes to develop the theoretical and computational tools necessary to take into account polaronic effects in GW in a full ab initio way. This theory will be implemented in the computer code abinit, and then benchmarked for simple and well-studied materials.

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\(^1\) L. Hedin, Phys. Rev. 139, A796-A823 (1965).