# O.11 Constrained DFT to mimick thermalized photo-excited carriers

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A number of materials have been recently reconsidered for their interaction with light. For instance, how ferroelectric materials change shape under illumination have attracted a lot of attention [1,2]. Most accurate methods to deal with the interaction of light and solids, such as solving the Bethe-Salpether equation, are very computationally intensive. As a result, it becomes extremely difficult to relax the structure under illumination. Here, we describe a simple method, in which we constrain n electrons to be excited across the bandgap in the conduction bands at each SCF iteration (see Figure 1) [3,4]. Those excited carriers are described by a Fermi-Dirac distribution with its own chemical potential, separate from the one of excited holes in the valence band. This is typically the description employed in modelling the thermalized photo-excited electrons and holes in pn-junction. Here we describe the principle of the implementation in abinit v9.4, and detail its application to a few problems, including photostriction in ferroelectric materials and photo-induced phase transition [4,5].

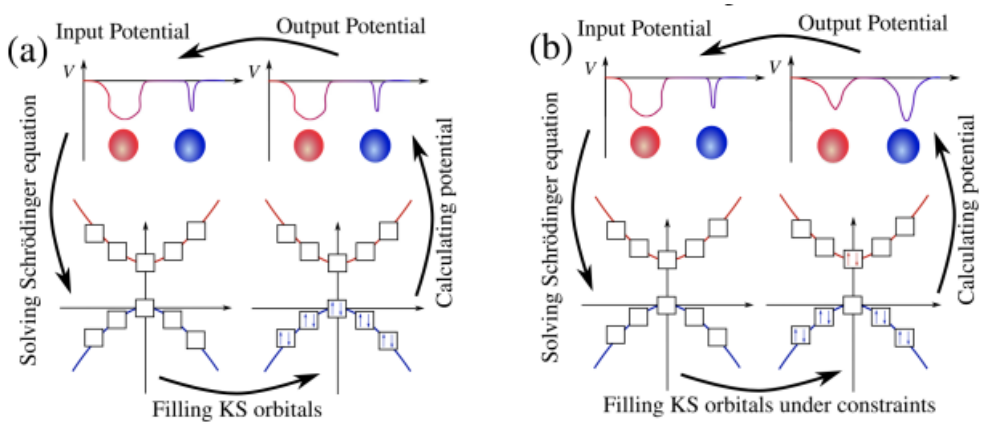


Figure O.1: (a) Ground state DFT in the Kohn-Sham (KS) ansatz, in which the lowest KS orbitals are filled to determine the output potential; (b) constrained DFT in which 2 electrons are constrained in the conduction band during the SCF cycle.

[1] B. Kundys *et al.*, *Nat. Mater.* **9**, 803 (2010).

[2] B. Kundys, *Appl. Phys. Rev.* **2**, 011301 (2015).

[3] Y. Yang *et al.*, *J. Phys. Condens. Matter* **30**, 073001 (2018).

[4] C. Paillard *et al.*, *Phys. Rev. Lett.* **123**, 087601 (2019).

[5] C. Paillard *et al.*, *Phys. Rev. Lett.* **116**, 247401 (2016).