Implementation of the LDA-1/2 method in ABINIT

F. Jollet$^1$ and G. Zéra$h^1$

$^1$ CEA DAM-DIF, F-91297 Arpajon, France

In this talk, we shall present the implementation of the LDA-1/2 method in ABINIT. We shall first mention the interest of the method to recover the band gap of semiconductors and show rapidly how it works [1]. We then shall detail the implementation in ABINIT, the keywords to be activated and the modifications introduced in the JTH table to account for this method. An example of a calculation in ABINIT will be shown at the end.

References