

Implementation of the LDA-1/2 method in ABINIT

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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

- [1] L. G. Ferreira, M. Marques, and L.K. Teles. Approximation to density functional theory for the calculation of band gaps of semiconductors. *Phys. Rev. B*, 78:125116, 2008.