O.3 Simulation of small polarons using ABINIT and functionalities related to correlated electrons

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Small polarons are additional electrons or holes in an insulator, that localize on a single atom due to a phenomenon called self-trapping. These additional charges are usually the result of the presence of donor (for electron polarons) or acceptor (for hole polarons) point defects. Their simulation in the framework of Density Functional Theory (DFT) necessitates, in general, to go beyond the local or semi-local functionals, because of the self-interaction error inherent to these functionals, that strongly disfavors localized states with respect to delocalized ones. In this talk, we will focus on how to simulate small polarons using DFT+U, and in particular how to use some specific functionalities present in the ABINIT code and related to DFT+U (control of occupation matrices of correlated orbitals), in order to obtain a very fine description of small polarons: how to localize a polaron on a desired atom in a supercell, and in a desired orbital, how to simulate polaron transfer and onsite reorientation [1]. The choice of U to describe small polarons will be discussed [2]. Applications will be shown on electron and hole polarons in several oxides.

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[1] G. Geneste, B. Amadon, M. Torrent, and G. Dezanneau, Phys. Rev. B **96**, 134123 (2017).

[2] M. Cococcioni and S. de Gironcoli, Phys. Rev. B **71**, 035105 (2005).