

## Automatize a DFT code: high-throughput workflows for Abinit

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**Abstract:** In the last years the increase of available computing power and the demand for large amount of data has highlighted the need for reliable ways of running DFT codes in an automated way. However, high-throughput DFT calculations in general require a robust framework to handle the whole process, from generating inputs to storing the final results, passing for the management of complex workflows. In order to bring a DFT code to the high throughput scale and prepare reliable and reusable workflows several challenges should thus be faced. Here, I will present the steps that have allowed to automatize the calculations with Abinit[1] thanks to the development and integration of several frameworks. In particular, I will focus on the aspects concerning the realization of the workflows based on the Fireworks[2] framework and on their application for the calculation of phonon band structures using Density Functional Perturbation Theory(DFPT)[3].

### **References:**

- [1] Gonze et al., Comput. <https://www.abinit.org> Phys.Commun.205,106-131(2016).
- [2] Jain et al., Concurrency and Computation: Practice and Experience 27,5037 (2015).
- [3] Petretto et al., Sci Data 5,180065 (2018).