

# Updates on high-throughput DFPT

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High-throughput calculations in general require a robust framework to handle the whole process from generating inputs to storing the final results. This is even more true in the case of Density Functional Perturbation Theory, where a large number of calculations should be performed to reach the final result.

The framework for high-throughput workflows with Abinit have been finalized and employed to generate full phonon band structures for more than 1500 materials in collaboration with the Materials project [1, 2]. The results will be shown along with a discussion of the problems that emerged running the calculations.

## References

- [1] A. Jain, S.P. Ong, G. Hautier, W. Chen, W.D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, K.A. Persson. The Materials Project: A materials genome approach to accelerating materials innovation, *APL Materials*, 2013, 1(1), 011002.
- [2] G. Petretto, S. Dwaraknath, H.P.C. Miranda, D. Winston, M. Giantomassi, M.J. Van Setten, X. Gonze, K.A. Persson, G. Hautier, G.-M. Rignanese, *Sci. Data* 5, 180065 (2018).