

AbiPy - An overview

M. Giantomassi¹ and the AbiPy developers

¹ Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Belgium

AbiPy is a python package that provides a flexible scripting environment for the analysis and the post-processing of ABINIT calculations as well as tools for the automatic generation of input files and the submission of jobs on parallel architectures. Started out as a mere set of scripts to automate the typical tasks needed during software development, AbiPy evolved gradually into a much more powerful and user-friendly toolkit that has been successfully employed in different domains including high-throughput DFPT applications [1], automatic *GW* calculations [2], generation and validation of pseudopotentials [3] as well as more conventional ab-initio studies [4]. In this talk, I will give an update on the new features available in version 0.6 and a brief description of the developments planned for the forthcoming releases.

References

- [1] G. Petretto *et al.*, *Sci. Data* **5**, 180065 (2018)
- [2] M. J. van Setten *et al.*, *Phys. Rev. B* **96**, 155207 (2017)
- [3] M. J. van Setten *et al.*, *Comput. Phys. Commun.* **226**, 39-54 (2018)
- [4] Y. Gillet *et al.*, *Sci Rep* **7**, 7344 (2017)