AbiPy - An overview

M. Giantomassi and the AbiPy developers

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