

AiiDA-SIESTA INTERFACE PRODUCT DETAILS



DESCRIPTION

The **siesta** program is able to perform, in a single run, the computation of the electronic structure, the optional relaxation of the input structure, and a final analysis step in which a variety of magnitudes can be computed: band structures, projected densities of states, etc.

FRAMEWORK

The operations to be carried out are specified in a very flexible input format. The AiiDA-SIESTA interface has been designed to run the most general SIESTA calculations through the **AiiDA** workflows, with support for most of the available options (limited only by corresponding support in the parser).



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