

GINESTRA-AiiDA INTERFACE PRODUCT DETAILS



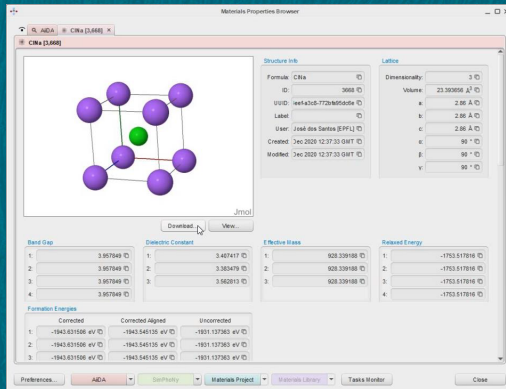
DESCRIPTION

The INTERSECT Ginestra-AiiDA interface is conceived to exchange European Materials Modelling Ontology (EMMO) compliant data from/to the AiiDA database in both the Material-To-Device (M2D) and Device-To-Material (D2M) workflows.

Its realization has represented one main step toward the implementation of the syntactic interoperability and the realization of the simulation Hub (sHub) of the Interoperable Material-To-Device (IM2D), as it allows for the interconnection via AiiDA of the device (GINESTRA) and of the materials (siesta,  codes.

FRAMEWORK

For M2D workflow, it is possible to retrieve/import a crystalline structure, retrieve a physical property, or submit/monitor the property computation. In case of D2M, the interface queries the AiiDA database via the REST-API, looking for the materials that match the outputs of the first block. Query may be refined according to specific filters: candidate materials list, variability range for the parameter, concatenation of multiple conditions (e.g., the material should satisfy both the band-gap and the dielectric constant values).



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