
aiida-symmetry-representation Documentation

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`aiida-symmetry-representation` is a plugin for AiiDA to run the `symmetry-representation` code. It implements a calculation and parser which allow for filtering the symmetries which are compatible with a given structure.

1.1 Calculation classes

class `aiida_symmetry_representation.calculations.filter_symmetries.FilterSymmetriesCalculation`
Calculation class to run the `symmetry-repr filter_symmetries` command.

Parameters

- **symmetries** (`aiida.orm.data.singlefile.SinglefileData`) – Set of all symmetries which are tested, in `symmetry-representation` HDF5 format.
- **structure** (`aiida.orm.data.structure.StructureData`) – Structure for which the compatibility of the symmetries is tested.

1.2 Parser classes

class `aiida_symmetry_representation.parsers.symmetries.SymmetriesParser` (*calc*)
Parses a symmetries file to an output file in `symmetry-representation` HDF5 format.

Returns `symmetries` – Output symmetries file.

Return type `aiida.orm.data.singlefile.SinglefileData`

CHAPTER 2

Indices and tables

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