
aiida-tools

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This package contains tools that make it easier to create calculations and workflows with AiiDA.

- *Installation*

CHAPTER 1

Installation

You can install this tool with pip:

```
pip install aiida-tools
```

1.1 Reference

This module contains general helper functions to aid in developing AiiDA calculations and workchains.

`aiida_tools.check_workchain_step(func)`

Decorator for workchain steps that logs (and re-raises) errors occurring within that step.

Contains default keyword arguments to pass classes as input to workchains.

`aiida_tools.workchain_inputs.WORKCHAIN_INPUT_KWARGS = {'serializer': <function get_fullname>}`

Keyword arguments to be passed to `spec.input` for serializing an input which is a class / workchain into a string.

`aiida_tools.workchain_inputs.get_fullname(cls_obj)`

Serializes an AiiDA workchain or workfunction to an AiiDA String. For workchains the class identifier is used, workfunctions are serialized in YAML format.

Parameters `cls_obj` (*WorkChain, workfunction*) – Object to be serialized

`aiida_tools.workchain_inputs.load_object(cls_name)`

Loads the workchain or workfunction from the serialized string.

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