AiiDA-QE INTERFACE PRODUCT DETAILS

DESCRIPTION

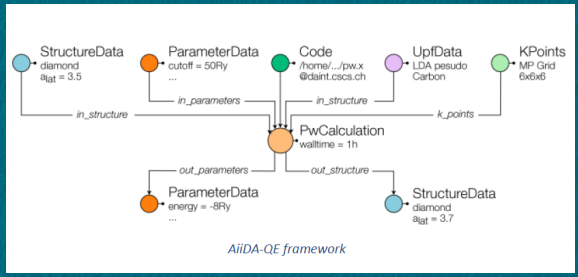
The AiiDA-QE interface permits accessing and automatically controlling (through AiiDA) the execution of complex quantum mechanical calculations performed with the QE suite.

QUANTUM ESPRESSO is a suite of open-source codes for electronic-structure calculations from first principles, based on Density-Functional Theory (DFT), plane waves, and pseudopotentials.

FRAMEWORK

Currently supported codes are:

- PW: Ground state properties, total energy, ionic relaxation, molecular dynamics, forces, etc.;
- CP: Car-Parrinello molecular dynamics;
- PP: Electronic structure analysis;
- PH: Phonons from density functional perturbation theory;
- TDDFPT: EELS and UV-vis absorption spectroscopy;
- GWW: many-body corrections;
- X-spectra: X-ray spectroscopy;
- Nudget Elastic Band (NEB): transition state barrier.



AiiDA-QE framework

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intersect-project.eu intersect@nano.cnr.it