

## **Materials Cloud three-dimensional crystals database (MC3D)**

This is a curated set of relaxed three-dimensional crystal structures based on raw CIF data taken from the external experimental databases MPDS, COD and ICSD. The raw CIF data have been imported, cleaned and parsed into a crystal structure; their ground-state has been computed using the SIRIUS-enabled pw.x code of the Quantum ESPRESSO distribution, and tight tolerance criteria for the calculations using the SSSP protocols.

This entire procedure is encoded into an AiiDA workflow which automates the process while keeping full data provenance. Here, since the original source data of the ICSD and MPDS databases are copyrighted, only the provenance of the final SCF calculation on the relaxed structures can be made publicly available.

The MC3D ID numbers come from a list of unique "parent" stoichiometric structures that has been created and curated from a collection of several experimental databases. Once a parent structure has been optimized using density-functional theory, it is made public and added to the online Discover section of the Materials Cloud (copyrights might prevent publishing the original parent). Note that since not all structures have been calculated, some ID numbers are missing from the public version of the database.

The full ID of each structure also contains as an appended modifier the functional that was used in the calculations. Since the ID number points to the same unique parent, mc3d-1234/pbe and mc3d-1234/pbesol have the same starting point, but have been then relaxed according to their respective functionals.