InfoMaticA

Rapid access to reliable experimental data is the foundation of materials science and technology. For atomic-scale understanding and simulations, crystallographic structural data are pivotal. To this end, the InfoMaticA component provides search and retrieval capabilities of the world's most comprehensive crystallographic structural databases of inorganic materials. The databases as listed below can be licensed from Materials Design and are delivered as integral part of the MedeA software.

Databases compiled from published work

- Inorganic Crystal Structure Data (**ICSD**) database from the Fachinformationszentrum Karlsruhe, Germany.
- **Pearson's data file**, which is being developed by Material Phases Data Systems (MPDS) under the direction of Pierre Villars, Switzerland; Pearson's data file is licensed from ASM International.
- **Pauling Data File** Binaries Edition is licensed from MPDS. In addition to structural data this database also contains phase diagrams
- NIST Crystal Data (**NCD**)

Together these databases represent the world's most comprehensive compilation of known inorganic crystal structures.

Collectively there are over 500,000 entries in these databases with approximately 100,000 unique inorganic crystal structures.

User-created databases

- The "MD" database allows users to store structural data, which can be the result of simulations performed with one of MedeA's simulation programs.

InfoMaticA allows the simultaneous search in all of these databases including the user-created databases. In the case of data from published results (e.g. from Pearson's or ICSD), InfoMaticA displays the bibliographic reference and explanatory text. The structures can be retrieved, viewed, and manipulated within the graphical user interface of MedeA. This includes the possibility to compute and display x-ray powder patterns.

The retrieval of crystal structures from one of the databases is often the first step in the modeling of a material. In fact, the agreement of computed and experimental lattice parameters and atomic positions of pure systems is an excellent initial test of the validity of a chosen computational approach.