MPOD: a Material Property Open Database linked to structural information

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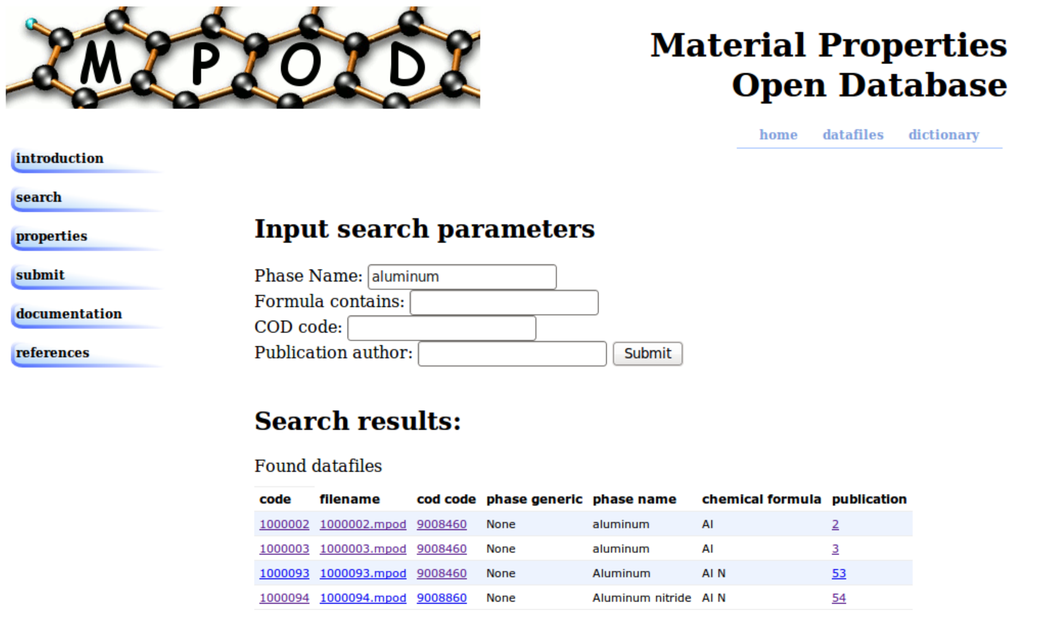
MOTIVATION

Crystallographic structures affect microscopic properties of the phases constituting a given material which has consequences at the macroscopic scale. Knowledge about the structure can also be used to make predictions about such properties, e.g. with a simulation approach (DFT, Molecular dynamics, …). Knowledge about experimentally measured crystallite properties, however, is of key importance for counter-checking theoretical studies and also to better define fitting models for the structure determination itself.



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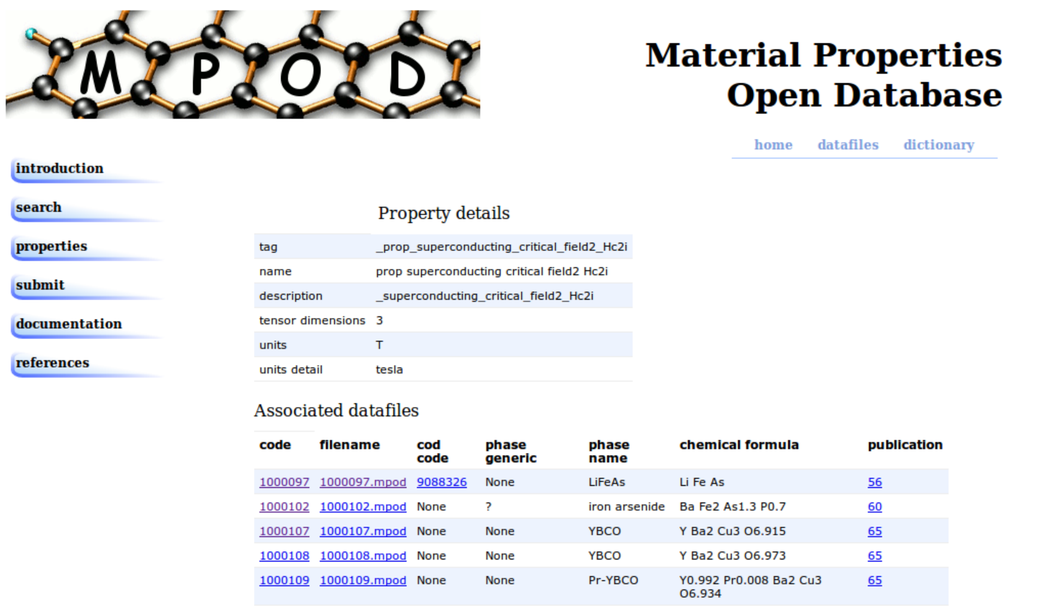
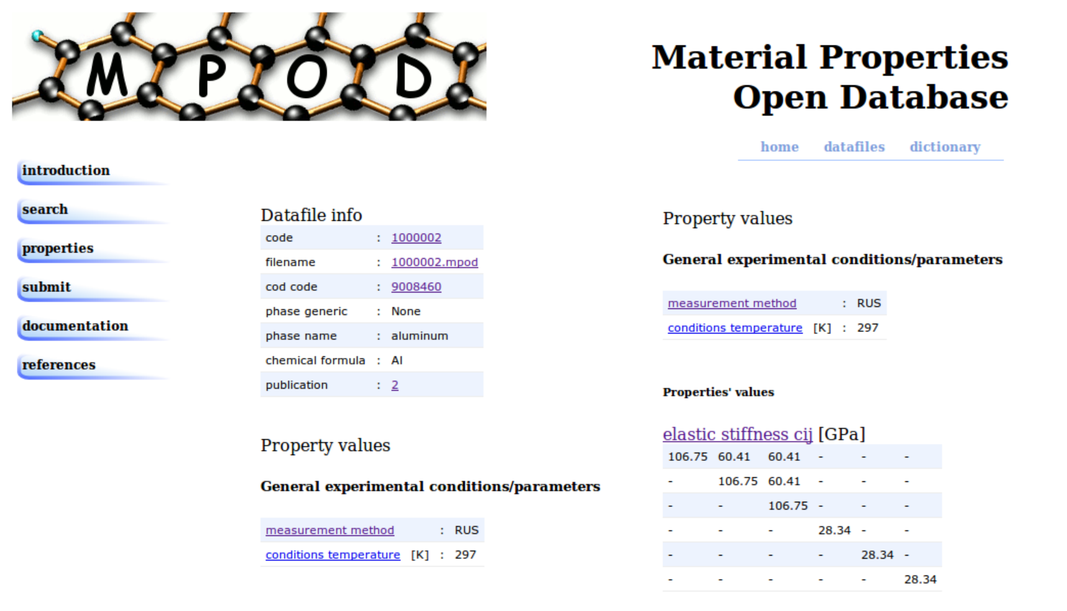
www.materialproperties.org





DISCUSSION and CONCLUSION

Inspired by the Crystallography Open Database, the Material Properties Open Database (MPOD) was given birth. MPOD aims at collecting and making publicly available at no charge tensorial properties (including scalar properties) of phases and linking such properties to structural information of the COD when available. MPOD files are written with the STAR file syntax, used and developed for the Crystallographic Information Files. A dictionary containing new definitions has been written according to the Dictionary Definition Language DDL1, although some tricks were adopted to allow for multiple entries still avoiding ambiguousness.\\

The initial set includes mechanical properties, elastic stiffness and compliance, internal friction; electrical properties, resistivity, dielectric permittivity and stiffness, thermodynamic properties, heat capacity, thermal conductivity, diffusivity and expansion; electromechanical properties, piezoelectricity, electrostriction, electromechanical coupling; optical properties; piezooptic and photoelastic properties; superconducting properties, critical fields, penetration and coherence lengths.\\

Properties are reported in mpod files where the original published paper containing the data is cited and structural and experimental information is also given. One mpod file contains information relative to only one publication and one phase.\\

A significative set of experimental parameters and measurement methods are included in the dictionary.

The website provides not also the files but also the dictionary and information on the software used for the syntactic correctness of the files. Further validation algorithms will be implemented in the near future taking into account the validity of the matrix indeces.

The work has already been presented at conferences and has received appreciations and interest. The advantage for the authors in fact is visibility of their work and data that can be searched through the web interface of the MPOD.

The website in fact provides reader-friendly views of the properties values, with links to the properties' definitions and the details of the publication where the data are released. A form for submitting new MPOD files will be put online in the near future.

Acceptance of contributions at international conferences and academic collaborations show the scientific relevance of the activity carried out.

Acknowledgement
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