

MPOD: a Material Property Open Database linked to structural information.

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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.

Inspired by the Crystallography Open Database (COD) a Material Properties Open Database (MPOD) was given birth. MPOD aims at collecting and making publicly available at no charge tensorial properties (then including properties represented by scalars) of phases and linking such properties to structural information contained in the COD. As its inspirator, MPOD files use a Starfile syntax used and developed for the Crystallographic Information Files (CIF). A dictionary containing new definitions has been written according to the Dictionary Definition Language DDL1. However some tricks were adopted to adapt the relatively strict Starfile syntax 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.

The files and the information therein contained can also be consulted on-line at www.materialproperties.org.

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