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The Representation of Physical Properties in the Material Properties Open Database (MPOD)

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The Material Properties Open Database (MPOD, http://mpod.cimav.edu.mx) is a functional element of the web-based *open databases* system linked with Crystallography. MPOD delivers single-crystal tensor properties in several representations, ranging from numerical matrices to 3D printing. Longitudinal moduli surfaces can be displayed in computers as well as in smart cell phones. Properties are stored as ".mpod" files. IUCr formatting standards (CIF) are followed. The original paper containing the data is cited. Structural and experimental information is also registered and linked. The MPOD system includes a physical properties dictionary with pertinent constitutive equations respecting Vol. D of the International Tables when possible. "Coupling properties", e.g. piezo-effects and magnetoelectricity, represent interactions linking different subsystems in a material. The implications of crystal symmetry in physical properties are systematically taken into account. Matrices' elements and longitudinal moduli surfaces are checked for consistency with the Neumann Principle. The representation of magnetic coupling properties and their link with magnetic symmetry concepts represent newly added features of MPOD. Color-symmetry and time-inversion considerations add complexity and interest to the task of systematizing the reception, validation and representation of this family of properties. The representation of polycrystals' properties constitutes a current challenge for the MPOD international group. Work on the systematization of the Voigt, Reuss and Hill approximations is described. The MPOD presentation includes a real-time demonstration of the database possibilities. Funding from Project CONACYT 257912 is acknowledged.

References:

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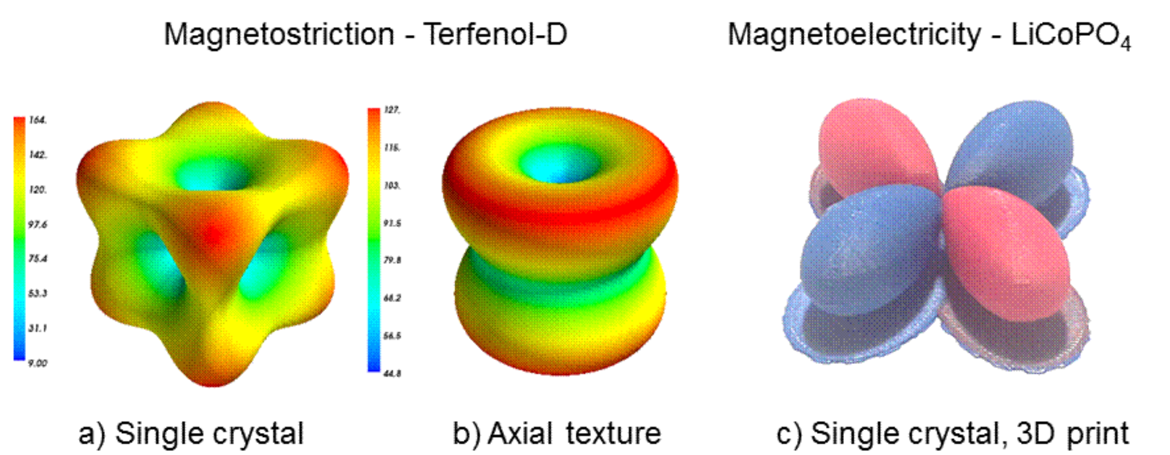

Figure 1: Longitudinal surface representations of Terfenol-D magnetostriction (a, b) and $LiCoPO_4$ magnetoelectricity (c).