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Software for the Characterization of Polycrystalline Compounds

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Innovative methodologies have been developed and implemented in computer programs aiming at providing efficient computational tools for a wide range of applications in the field of the characterization of polycrystalline materials. The software, based on sound theoretical principles, developed according to the most recent and advanced programming languages and supported by a high level of automatism which makes its use simple also to non-expert in crystallographic knowledge, is worldwide used.
The developed software are:
EXPO1: a computing program devoted to structure solution of materials available in the form of microcrystalline powder, by using X-ray diffraction data. The chemical formula and the experimental diffraction profile are the only information necessary to run it. EXPO is able to investigate small molecules, inorganic, organic and metal-organic. It can execute, in a complete automatic way, all the steps characterizing the structure solution process and consisting of: 1) identification of crystal cell parameters; 2) determination of space group; 3) solution of crystal structure by locating the correct atom positions; 4) refinement of the final crystal model.
QUALX2: a software for identifying the crystal phase(s) present in a powder sample. It automatically performs: 1) the location of peaks in the experimental diffraction profile, 2) the subtraction of the background noise, 3) the search in crystal phase databanks. At the end of the process, QUALX brings out the chemical phase(s) which best match the peaks in the experimental pattern. In addition, it can query two databases: one commercial (PDF-2) and one free (POW_COD).
OChemDb3(Open Chemistry Database): a new free web portal which has been developed for assisting in the crystal structure determination process by searching and analyzing crystal chemical information of organic and inorganic compounds. OChemDb is dedicated to collect, to make available by statistical tools and to manage crystal-chemical information coming from the CIF files contained in the Crystallography Open Database (COD, http://www.crystallography.net/cod/). OChemDb can be used for searching and analyzing crystal-chemical information (bond distance, bond angle, space group) of structures already solved, to be used for different scientific purposes. It provides statistics on desired distances, bond angles, torsion angles and space groups. OChemDb uses a suitably designed database of solved crystal structures. The use of OChemDb requires only a web browser and an internet connection.
For each software, examples of challenging applications by users around the world covering a wide range of scientific interests will be presented.

Primary authors: Dr CORRIERO, Nicola (CNR - Istituto di Cristallografia); Dr ALTOMARE, Angela (CNR - Istituto di Cristallografia); Dr CUOCCI, Corrado (CNR - Istituto di Cristallografia); Dr FALCICCHIO, Aurelia (CNR - Istituto di Cristallografia); Dr RIZZI, Rossana (CNR - Istituto di Cristallografia)

Presenter: Dr CORRIERO, Nicola (CNR - Istituto di Cristallografia)

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