Page 1

Crystallography Open Database (COD), Predicted Crystallography Open Database (PCOD) and Material Properties Open Database (MPOD)

Saulius Gražulis^a, Giancarlo Pepponi^b, Justas Butkus^a, Andrius Merkys^a, Adriana Daškevič^a, Armel Le Bail^c, Robert Downs^d, Luca Lutterotti^e, Peter Moeck^f, Miguel Quirós Olozábal^g, <u>Daniel Chateigner^h</u>

a Vilius University Institute of Biotechnology, Vilnius, Lithuania b Fondazione Bruno Kessler, Trento, Italia c Laboratoire des Oxydes et Fluorures, CNRS and Université du Maine, Le Mans, France d Department of Geosciences, University of Arizona, Tucson, Arizona, USA e Department of Materials Engineering, University of Trento, Trento, Italy f Portland State University, Department of Physics, Portland, Oregon, USA g Departamento de Química Inorgánica, Universidad de Granada, Granada, Spain h CRISMAT-ENSICAEN, IUT-Caen, Université de Caen Basse-Normandie, Caen, France daniel.chateigner@ensicaen.fr

Opening scientific data to the largest community, an intrinsic goal of any researcher, is becoming real with the advent of intensive use of internet. However, researchers' dedication to fundamental and applied research only allocate little spare time to this. The only way to achieve the goal is to involve as many volunteers as possible willing to help, and to automate uploading procedures.

We achieved this in the Crystallography Open Database (www.crystallography.net) and Predicted Crystallography Open Database (http://www.crystallography.net/pcod/index.html) for some years to date, with a growing number of crystallographic information files (more than 118000 and 10⁶ items respectively), and uploading automation ready for use and for further developments. Mirroring on several servers worldwide guarantees the open character of the databases and the availability of data.

Feedbacks from many colleagues worldwide, teachers and researchers, strongly encourage our approach. Moreover, several crystallography-related renown companies now use the COD and PCOD databases in their own software, adding much value to the original idea.

Very recently, because several aspects of crystallographic calculations require intrinsic material properties, we launched the Material Properties Open Database (<u>http://www.materialproperties.org/</u>). This latter sister database collects tensorial properties of any rank and for any phase, linked, when possible, to structure information in the COD database.

The presentation aims at showing the actual development states of the three databases and their functionalities.