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Internet Based Open Access Crystallographic Databases GIRISH UPRETI,

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ERN SEIPEL, MORGAN HARVEY, WILL GARRICK, PETER MOECK, Portland State University — Two freely accessible crystallographic databases are discussed: the Crystallographic Open Database (COD, http://crystallography.net) which contains over 37,000 crystal structures, and the Nano-Crystallography Database (NCD, http://nanocrystallography.research.pdx.edu) which we recently started to support image-based nanocrystallography and (nano) materials science education. Both databases collect crystallographic relevant information in a standardized format; the Crystallographic Information File (CIF). CIF is the standard file format adopted by the International Union of Crystallography (http://iucr.org) for the archiving and distribution of crystallographic information. A subset of the COD, the Predicted Crystallographic Online Database, allows for 3D structural displays of structural polyhedra and wireframes of approximately 2,600 entries. Since electron microscopist are interested in simple, yet technologically important materials, the crystallographic information for those materials will be included in our database. At our NCD site, entries in the COD and the NCD can be visualized in three dimensions (3D) along with (2D) lattice fringe fingerprints plots. The latter supports the identification of unknown nanocrystal phases from high-resolution transmission electron microscopy (HRTEM) images. Morphological crystal information from the database "Bestimmungstabellen für Kristalle/????????????????," (A.K. Boldyrew and W.W. Doliwo-Dobrowolsky, Zentrales Wissenschaftlichers Institute der Geologie und Schürfung, Leningrad/ Moscow, 1937/1939) will also be included in the NCD to support image-based nanocrystallography in 3D.

> Girish Upreti Portland State University

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