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High-Throughput Identification of Unique Structure Prototypes in the Inorganic Crystal Structure Database DAVID HICKS, CORMAC TOHER, OHAD LEVY, STEFANO CURTAROLO, Duke Univ — High-throughput computational assessment of materials properties is currently a major component of the effort to develop new useful materials by uncovering trends and correlations between structures, compositions, and functionalities. Efficient implementation of this approach thus requires a systematic identification of distinct material structure prototypes. We have developed a robust algorithm that calculates the level of similarity between crystal structures independent of the unit cell representation, using the comparison method proposed by Burzlaff [1]. This algorithm has been implemented in the high-throughput framework, Automatic Flow (AFLOW) [2], and applied to the Inorganic Crystal Structure Database (ICSD) [3] entries in the AFLOWLIB.org [4] online repository. We have determined the uniqueness statistics for the ICSD and have created a comprehensive set of the unique structural prototypes represented in it. [1] H. Burzlaff and Y. Malinovsky Acta Cryst. A53, 217-224 (1997). [2] S. Curtarolo et al. Comp. Mater. Sci. 58, 218-226 (2012). [3] FIZ Karlsruhe and NIST, Inorganic Crystal Structure Database, http://icsd.fiz-t karlsruhe.de/icsd/ [4] S. Curtarolo et al. Comp. Mater. Sci. 58, 227-235 (2012).

David Hicks
Duke Univ

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