Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

AFLOWSYM: A robust procedure to perform the complete symmetry analysis of crystals DAVID HICKS, COREY OSES, Dept. of Mechanical Engineering and Materials Science, Duke University, STEFANO CURTAROLO, Materials Science, Electrical Engineering, Physics and Chemistry, Duke University — Determination of the symmetry profile of structures is a persistent challenge in materials science as evident from implementation-specific results. Herein, we present a robust procedure for evaluating the complete suite of symmetry operations, including that of the lattice point group, factor group, crystallographic point group, and space group. The protocol resolves a system-specific mapping tolerance, which accounts for variability of error in reported atomic positions. A tolerance is validated through an analysis of the operations it defines, which must all be consistent with fundamental crystallographic principles. The approach has been successfully tested against the Inorganic Crystal Structure Database (ICSD) [1] entries cataloged in the aflow.org [2] online repository. The AFLOWSYM package is implemented within the automatic, high-throughput computational framework AFLOW [3] and is available for public use at aflow.org [3]. [1] FIZ Karlsruhe and NIST, Inorganic Crystal Structure Database, http://icsd.fiz-karlsruhe.de/icsd/ [2] S. Curtarolo et al. Comp. Mater. Sci. 58, 227-235 (2012). [3] S. Curtarolo et al. Comp. Mater. Sci. 58, 218-226 (2012).

David Hicks
Dept. of Mechanical Engineering and Materials Science, Duke University

Date submitted: 11 Nov 2016 Electronic form version 1.4