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The New NRL Crystallographic Database[1] MICHAEL MEHL, Naval Research Laboratory, Washington DC 20375, STEFANO CURTAROLO, DAVID HICKS, CORMAC TOHER, Duke University, Durham, NC, OHAD LEVY, Duke University, Durham, NC and NRCN, Israel, GUS HART, Brigham Young University, Provo, Utah — For many years the Naval Research Laboratory maintained an online graphical database of crystal structures for a wide variety of materials. This database has now been redesigned, updated and integrated with the AFLOW framework for high throughput computational materials discovery (http://materials.duke.edu/aflow.html). For each structure we provide an image showing the atomic positions; the primitive vectors of the lattice and the basis vectors of every atom in the unit cell; the space group and Wyckoff positions; Pearson symbols; common names; and Strukturbericht designations, where available. References for each structure are provided, as well as a Crystallographic Information File (CIF). The database currently includes almost 300 entries and will be continuously updated and expanded. It enables easy search of the various structures based on their underlying symmetries, either by Bravais lattice, Pearson symbol, Strukturbericht designation or commonly used prototypes. The talk will describe the features of the database, and highlight its utility for high throughput computational materials design.

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