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Enhancing AFLOW Visualization using Jmol JACOB LANASA, ELIZABETH NEW, PATRIK STEFEK, BRIGETTE HONAKER, ROBERT HANSON, St. Olaf College, AFLOW COLLABORATION — The AFLOW library[1,2] is a database of theoretical solid-state structures and calculated properties created using high-throughput *ab initio* calculations. Jmol[3] is a Java-based program capable of visualizing and analyzing complex molecular structures and energy landscapes. In collaboration with the AFLOW consortium, our goal is the enhancement of the AFLOWLIB database through the extension of Jmol's capabilities in the area of materials science. Modifications made to Jmol include the ability to read and visualize AFLOW binary alloy data files, the ability to extract from these files information using Jmol scripting macros that can be utilized in the creation of interactive web-based convex hull graphs, the capability to identify and classify local atomic environments by symmetry, and the ability to search one or more related crystal structures for atomic environments using a novel extension of inorganic polyhedron-based SMILES strings. [1] S. Curtarolo, *et al.*, *AFLOW: an automatic framework for high-throughput materials discovery*, Comp. Mat. Sci. **58**, 218-226 (2012). [**doi=10.1016/j.commatsci.2012.02.005**]; [2] S. Curtarolo, *et al.*, *AFLOWLIB.ORG: a distributed materials properties repository from high-throughput ab initio calculations*, Comp. Mat. Sci. **58**, 227-235 (2012). [**doi=10.1016/j.commatsci.2012.02.002**]; [3] R. Hanson, *Jmol – A Paradigm Shift in Crystallographic Visualization,* J. Appl. Cryst. **2010** *43*, 1250-1260.

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