

Poster Presentations

[MS41-P06] DRAWxtl 5.6 -An open-source program for crystal structure drawings.

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DRAWxtl[1] is a free and open-source drawing program that supports all the conventional elements of crystal structure drawings such as atomic spheres, thermal displacement ellipsoids and coordination polyhedra of arbitrary complexity. Additional graphical features include lone electron pair cones, magnetic moment arrows and mesh or solid-surface representations of electron density that can be combined with color-coded cross-sectional plots. While the origins of the program date back two decades now, it is still under active development by its original authors. A distinctive feature of DRAWxtl is its capability to handle composite and modulated crystal structures up to 3+3D natively, with full interactive control over the t and x parameter(s) and optional scaling of sphere radii with site occupancy numbers. Walk-throughs of configuration space can also be saved as movies. Although it is mainly designed for the rendering of experimental inorganic crystal structure data, with import filters for CIF, CSD, Fullprof, GSAS, JANA and SHELX format, it is equally well suited for displaying the results of DFT calculations done with the popular VASP, WIEN2k and ELK codes. The new version 5.6 contains many improvements across the board, from support for new modulation functions introduced in recent updates to JANA2006, to a significant speedup in reading of electron density map files, improvements in drawing Bader surfaces and numerous enhancements in object rendering styles. Special attention has been put on the novel possibilities provided by the recent advances towards affordable, high-quality

printing of accurate 3D structural models. To this end, the long-since available VRML output has been improved and a new export option for the OpenSCAD package has been added to facilitate generation of industry-standard STL and AMF files for printing softwares and service providers that do not yet handle VRML sufficiently well. The program is freely available under the GPLv2 license from <http://www.lwfinger.com/drawxtl/> in the form of ready-to-run binaries for Linux, OS X and Windows, as well as in C++ source code form for building on other platforms.

[1] Finger, L.W., Toby, B.H. & Kroeker, M. (2007). *J. Appl. Cryst.* **40**, 188-192.

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