MS18-P3 **MoProViewer: a molecule viewer for the MoPro charge density analysis program.** Benoît Guillot, *Laboratoire de Cristallographie, Résonance Magnétique et Modélisations (CRM^2) UMR 7036 Université Henri Poincaré, Nancy (France).*
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The MoPro program suite [1] is a crystal structure and charge density refinement package which includes two main modules: the MoPro least-squares refinement program and VMoPro, a tool dedicated to the computation of properties derived from the electron density. MoPro already possesses its own graphical user interface, but VMoPro was still a text-based program. Hence we present MoProViewer: a molecule viewer designed as an interface to VMoPro, and thus especially dedicated to the field of charge density analysis. MoProViewer is written in C++ and is based on the Qt SDK and on the Armadillo [2] and OpenGL libraries. It will be released once published as free of charge and open-source software under the GNU-GPL license. MoProViewer offers a wide range of features, among which:

– Compatibility with the MoPro molecular file format (including exportation), and with all the other formats allowed by the MoPro conversion program (CIF, shelxl RES, XD …).
– Several molecule representation modes (lines, balls & sticks).
– All standard molecule viewer capabilities (configurable atoms labeling and atoms coloring scheme, images exportation).
– All standard crystal structure analysis tools (stereochemistry measurements, symmetry handling, thermal ellipsoids drawing).
– Representation and modification of multipolar model atomic axis systems and chemical equivalencies constraints.
– Setup and control of most of the VMoPro possible computations (electron densities, electrostatic potentials, $\rho(r)$ topology …).
– Representation of the properties computed by VMoPro, or readable in XPLOR or Gaussian CUBE format, as 3D isosurfaces, 2D isocontours plots, 3D gradient lines or 2D slices of scalar fields.
– Possibility to color any isosurface on the basis of values of any other loaded scalar field using texture mapping method.
– Drawing of critical points and bond paths obtained from an electron density topology analysis.
– A powerful atom selection tool allowing easy computation focusing on any fragments or regions of a molecule, which is especially convenient in case of large structures (proteins).
– Handling of transferable electron density parameters database.
– Computation and representation of electron density topological basins in the AIM theory.

[1] Jelsch, C., Guillot, B., Lagoutte, A. & Lecomte, C. (2005) *J. Applied Cryst.* **38**, 38-54.
[2] Sanderson, C. (2010) "Armadillo: An Open Source C++ Linear Algebra Library for Fast Prototyping and Computationally Intensive Experiments" *NICTA Technical Report*.

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MS18-P4 **Mosaic Structure of Single Crystals: Investigation of Mosaicity and Anisotropy of Pyrite.** Anne K. Hüsecken,[a] Semen Gorfman[a] and Ullrich Pietsch[a] [a]*Universität Siegen, Germany*
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Extinction is a long-standing problem in X-ray crystal structure analysis, occurring due to multiple scattering in crystals. Over the years several extinction correction theorems have been formulated, but the used parameters have never been proved to be valid for a certain crystal under investigation. The measured intensities of real crystals do not fulfil the kinematical ($I \sim |F|^2$) nor the dynamical theory ($I \sim |F|$). They are in between both cases and an extinction correction, y ($I \sim y|F|^2$) is needed to fulfil the kinematic approach.

Present theories of extinction in single crystals are based on the model of a mosaic crystal with different shapes and sizes of mosaic blocks. They describe intensities of X-ray diffraction in terms of the kinematical approach and using certain "correction terms" to implement the mosaic structure of a real crystal **[1, 2, 3]**. At the moment crystallographers use the extinction correction as a black box. They do not prove whether the extinction model used is valid or invalid because the parameters are typically not verified by the experiment.

The mosaic blocks within a real crystal are disorientated relative to each other and are also affected by a lattice strain. In addition both 3D shape and size of the blocks are not known. All these parameters can be determined by high-resolution X-ray diffraction techniques performing ω- and ω-2θ-scans through certain reciprocal lattice nods. The measured widths of these scans can be used as input parameters for a possibly anisotropic extinction correction model for the crystal under investigation.

The aim of this work is to test this approach for the case of a pyrite crystal. This material shows significant effect of extinction (up to 50%, **[4])** and is therefore an appropriate model system for our studies. Because pyrite shows an anisotropic mosaic block size, we can use the data with respect to an anisotropic extinction correction. Our approach is tested by comparing the electron density refinement based on experimental data with and without the improved extinction correction.

[1] Becker, P. J. & Coppens, P. (1974). *Acta Cryst.* A**30**, 129.
[2] Suortti, P. (1982). *Acta Cryst.* A**38**, 642.
[3] Zachariasen, W. H. (1967). *Acta Cryst.* **23**, 558.
[4] Templeton, D. H. & Templeton, L. K. (1992). *Acta Cryst.* A**53**, 6227.

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