



## Editorial

### Crystallography in Switzerland and elsewhere from 1912 to 2013 and beyond



Hans-Beat Bürgi

UNESCO has pronounced 2014 the International Year of Crystallography (<http://www.iycr2014.org/>)

The first article of this issue explains the importance of the event. It commemorates the revolution in our perception of the microscopic world, which was initiated by Laue in 1912 and by father and son Bragg in 1913. For the first time in natural history it became possible to 'see' atoms.

The history of crystal structure determination by X-ray or neutron diffraction is the story of an unprecedented scientific success: within 100 years the method has not only become one of the most important analytical techniques, but is now so well understood that it could be coded – almost completely – into suites of computer software that do the job more or less automatically for biomolecules, newly synthesized chemical compounds and materials. It is due to this success that 'Crystallography' is often used as a synonym for X-ray crystal structure determination, although the field of crystallography is of course much broader. It is best seen as an intersection of mathematics, mineralogy, physics, chemistry and molecular biology.



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Does all this success mean that crystallography is a mature branch of science in need only of periodically adapting experiments and their interpretations to the new technological developments, but not likely to produce important breakthroughs? Yes and no!

Admittedly: YES, routine crystal structure determination from Bragg reflections produces reliable structural models of nearly any molecule or chemical compound for which well-ordered crystals can be obtained. Nowadays every science faculty at the Swiss universities and a significant portion of the Swiss chemical industries profits from a crystallographic structure service that usually offers both single crystal and powder diffraction analysis and sometimes other characterization methods as well.

But also: NO, there is still a universe to discover for all those interested in the vast spaces between the Bragg reflections, for all those interested not just in the ideal average structure, but rather in real structures with their defects, faults and disorder, aspects which are often a prerequisite for interesting and useful materials properties. New, more efficient methods are badly needed to uncover these secrets.

And further: NO. While the atomic scale architecture of matter is revealed through the diffraction of X-ray, macroscopic structure is imaged through the absorption of X-rays as in a medical 'X-ray'. For the much less well-known intermediate region of nano- and meso-scale structural features the two approaches are combined into new methods, such as phase sensitive X-ray tomography and ptychography. There is a world of nano- and mesoscale features of biological tissues and technical materials to be discovered in order to better understand their functions.

In addition: NO, the quality of X-rays beams in terms of both intensity and coherence that is delivered by synchrotrons and soon by the free-electron laser SwissFEL, approaches that of visible laser light. Much of the frontier research mentioned in the two preceding paragraphs depends on or becomes possible only with such high-quality radiation. Even such mundane applications as medical 'X-rays' may profit in the long run. Frontier research requires and the new experiments produce enormous amounts of data. With the continuing increase in computing power, these data can now be handled efficiently and interpreted meaningfully.

In crystallographic research, as in other scientific research, it is becoming increasingly clear that the full potential of structure determination can only be realized by combining it with biological, physical or physicochemical experiments. Part of this research is exploring the fringes of crystallography itself including quasicrystals, disorder in crystals and the structure and chemistry at surfaces. Further areas of research include the planning of experiments with the SwissFEL such as powder diffraction, biocrystallography and fast kinetics. As in most other fields, new territory is best discovered starting from the frontiers of the known world.

The description above may evoke the impression of a lively Swiss crystallography scene. It is fool's gold! Much of the research hinted at above is done by solid-state physicists, physical chemists and – last but not least – crystallographers close to and beyond retirement. While it is necessary and healthy

to infuse fresh blood into a field that is 100 years old, the closing down of the Swiss crystallographic laboratories, still in existence 10 years ago, had serious repercussions on the crystallographic literacy of the main users of crystallographic techniques, namely students and postdocs in physics, mineralogy, chemistry and molecular biology. The crystallographic education of the science students has declined alarmingly and is now largely outsourced to summer schools, such as the Zürich School of Crystallography which takes place every second year at the University of Zürich at non-negligible cost for the students (<http://www.chem.uzh.ch/linden/zsc/>). Five of the school's ten tutors are primarily responsible for crystallographic service labs, three others are retired crystallographers.

The overview in this special issue is necessarily incomplete. The choice and omission of topics are entirely the responsibility of the editors. We hope that you, the readers of CHIMIA, will enjoy this mosaic display of crystallographic activities in Switzerland anyway.

We thank the Swiss Chemical Society for this opportunity to present the past and present as well as problems and future perspectives for crystallography in the sciences, a tool – one is tempted to say – that is second to none.

Hans-Beat Bürgi and Katharina Fromm

**Hans-Beat Bürgi** is professor emeritus at the University of Bern, permanent academic guest at the Department of Chemistry of the University of Zurich and visiting scientist at UC Berkeley. His main current research interest is the structure determination of disordered materials with interesting and useful properties from analyses of the diffuse scattering between the Bragg reflections. The work includes developing methods and corresponding software for this computationally demanding problem as well as studies of highly disordered materials such as molecular pigments and multivariate metal-organic framework compounds. Earlier research focused on molecular motion in crystals and on structure correlation, *i.e.* mapping of reaction path with structural snapshots extracted from crystal structures.

After a PhD in organometallic chemistry with Prof. E. Hey-Hawkins in Karlsruhe, and postdocs in solid state and supramolecular chemistry with Prof. J. Strähle in Tübingen and Prof. J.-M. Lehn in Strasbourg, respectively, **Katharina M. Fromm** became a maître-assistante in Geneva where she received her habilitation in 2002. She accepted an SNF-Professorship in Basel before moving to Fribourg in 2006, where she holds the chair in inorganic chemistry. Her research areas reach from antimicrobial coordination polymers to nanoscale electrode materials for Li-ion batteries, *via* mixed metal cluster compounds and nanocontainers for drug delivery, spanning thus her chemistry from materials science to biomedicine. In 2014, she will take the presidency of the Chemistry Platform of the SCNat, and she organizes, together with the Swiss and European Crystallographers the European Crystallography Meeting in Basel from August 28th – September 1st 2016.