

Acta Crystallographica Section A

**Foundations and
Advances**

ISSN 2053-2733

Celebrating the past, looking to the future

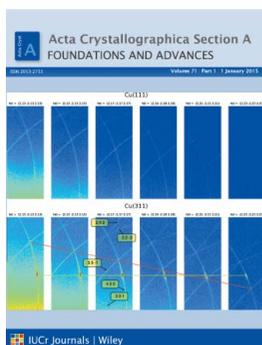
Simon J. L. Billinge and Jianwei Miao

Acta Cryst. (2015). **A71**, 1–2

Copyright © International Union of Crystallography

Author(s) of this paper may load this reprint on their own web site or institutional repository provided that this cover page is retained. Reproduction of this article or its storage in electronic databases other than as specified above is not permitted without prior permission in writing from the IUCr.

For further information see <http://journals.iucr.org/services/authorrights.html>



Acta Crystallographica Section A: Foundations and Advances publishes articles reporting fundamental advances in all areas of crystallography in the broadest sense. This includes metacrystals such as photonic or phononic crystals, *i.e.* structures on the meso- or macroscale that can be studied with crystallographic methods. The central themes are, on the one hand, experimental and theoretical studies of the properties and arrangements of atoms, ions and molecules in condensed matter, periodic, quasiperiodic or amorphous, ideal or real, and, on the other, the theoretical and experimental aspects of the various methods to determine these properties and arrangements. In the case of metacrystals, the focus is on the methods for their creation and on the structure–property relationships for their interaction with classical waves.

Crystallography Journals **Online** is available from journals.iucr.org

Celebrating the past, looking to the future

Simon J. L. Billinge^{a,b*} and Jianwei Miao^{c*}

^aDepartment of Applied Physics and Applied Mathematics, Columbia University, 200 Mudd, 500 W 120th Street, New York, NY 10027, USA, ^bCondensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973, USA, and ^cDepartment of Physics and Astronomy and California NanoSystems Institute, University of California, Box 951547, Los Angeles, CA 90095-1547, USA

It is with great excitement that we look forward to the New Year at *Acta Crystallographica Section A: Foundations and Advances*. As the International Year of Crystallography draws to a close, we were delighted to read in the *Nature* article *The top 100 papers* [Van Noorden, R., Maher, B. & Nuzzo, R. (2014). *Nature*, **514**, 550–553] that crystallography was well represented. We were even more excited to find that a full seven of the top 100 articles were published in IUCr journals, and of these, four were in *Acta A* (in the order in which they appear in the list):

(1) *A short history of SHELX* by G. M. Sheldrick [*Acta Cryst.* (2008). **A64**, 112–122];

(2) *Revised effective ionic radii and systematic studies of interatomic distances in halides and chalcogenides* by R. D. Shannon [*Acta Cryst.* (1976). **A32**, 751–767];

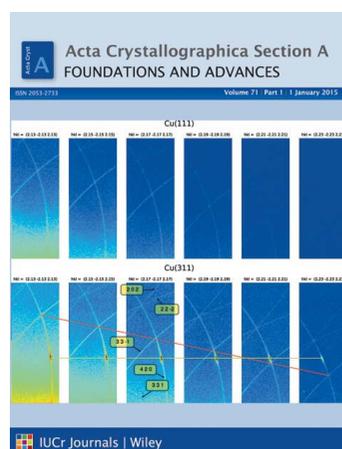
(3) *Phase annealing in SHELX-90: direct methods for larger structures* by G. M. Sheldrick [*Acta Cryst.* (1990). **A46**, 467–473]; and

(4) *Improved methods for building protein models in electron density maps and the location of errors in these models* by T. A. Jones, J.-Y. Zou, S. W. Cowan and M. Kjeldgaard [*Acta Cryst.* (1991). **A47**, 110–119].

The 2008 paper by George Sheldrick is No. 13 on the top 100 list and is the highest-ranked paper published in the past two decades. As of the end of 2014, it has had over 39 000 citations. This speaks to the enduring scientific (and societal) impact of crystallography even into the 21st century, and to the important place that *Acta A* has in this rich and ongoing history. We are obviously delighted that in this January 2015 edition of *Acta A* we publish, as one of our three *Advances* papers, Professor Sheldrick's paper describing *SHELXT*, a new weapon in the crystallographer's arsenal and a new member of the *SHELX* suite of programs [Sheldrick, G. M. (2015). *Acta Cryst.* **A71**, 3–8]. We believe that, moving forward, the contributions of crystallographers (and nano-crystallographers and non-crystalline crystallographers) will continue to be pivotal and have broad scientific reach, and we believe that *Acta A*'s wonderful tradition and position as the main foundational journal for advances in structure science will be maintained.

We would like to thank our editorial board, reviewers and authors for their hard work in 2014, the more so because striving for the highest standards, as we are, takes more care and application on everyone's part. We strongly believe that the hard work is worth it and that *Acta A* will go from strength to strength in 2015. The first *Advances* paper, *Magnetic pair distribution function analysis of local magnetic correlations* by B. Frandsen, X. Yang and S. J. L. Billinge [*Acta Cryst.* (2014). **A70**, 3–11], was published online in December 2013, exactly one year ago. In this January 2015 edition of the journal we have three *Advances* papers:

SHELXT – Integrated space-group and crystal-structure determination by G. M. Sheldrick [*Acta Cryst.* (2015). **A71**, 3–8];



Nuclear-weighted X-ray maximum entropy method – NXMEM by S. Christensen, N. Bindzus, M. Christensen and B. Brummerstedt Iversen [*Acta Cryst.* (2015). **A71**, 9–19]; and

Diffuse multiple scattering by A. G. A. Nisbet, G. Beutier, F. Fabrizi, B. Moser and S. P. Collins [*Acta Cryst.* (2015). **A71**, 20–25].

We are also receiving increasing numbers of submissions, for which we thank you. The standards for being published as an *Advance* are high, and include the broad appeal and potential impact of the work as well as its scientific correctness, but we hope that these papers will be seen as the gold standard for exciting new developments in structure science, which is why we offer accelerated review and production for *Advances* articles along with promotion after they are published. We encourage you to submit your best work to us for consideration as an *Advance*.

The *Advances* section will also be featuring a number of *Lead Articles* in 2015, in which well known experts will be providing useful overviews of different fields of research. We have several articles in the pipeline, including ones discussing electron crystallography of protein microcrystals, quantitative scanning transmission electron microscopy, the complementary nature of

powder diffraction and electron crystallography, and cryogenic coherent X-ray diffraction imaging of biological particles. Suggestions from our readers for topics for *Lead Articles* are also welcome.

Looking forward, we would like to expand the scope of *Acta A* and include some new directions, such as X-ray free-electron lasers (XFELs), various coherent diffractive imaging (CDI) methods (such as plane-wave CDI, Bragg CDI and ptychographic CDI), serial crystallography, aberration-corrected electron microscopy, electron and X-ray tomography, nanocrystallography, disorder in materials, dynamics and time-resolved experiments, and so on.

As we strive to keep *Acta A* at the forefront of developments in crystallography and structure science, we are adopting higher standards for acceptance of articles across the board. For example, beyond just describing a development, each article should identify the rationale for making the development and how it would be used by the crystallographic community, and we look forward to collaborating with our authors to bring this about.

Finally, we would like to wish all of our authors, editors, reviewers and readers a wonderful, prosperous, productive and happy 2015.