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► **To cite this version:**

Massimo Nespolo. The Everlasting Challenges of Mathematical and Theoretical Crystallography. 2020, pp.2000057. 10.1002/crat.202000057 . hal-02568041

HAL Id: hal-02568041

<https://hal.univ-lorraine.fr/hal-02568041v1>

Submitted on 11 May 2020

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The Everlasting Challenges of Mathematical and Theoretical Crystallography

Massimo Nespolo

The IUCr Commission on Mathematical and Theoretical Crystallography (MaThCryst) was established in 2005 after a three-year informal existence as an unofficial workgroup. The reasons for this initiative were essentially the need to draw new lymph in a field that was sliding away from our community, and to energize the education of young (and sometimes less young) crystallographers in the foundations that too often are overlooked in the University curricula. The task seemed extremely challenging, but despite some scepticism we had to face at first, our work has been successful from the beginning. Today we count more than fifty events (workshops, satellite conferences, schools) during our fifteen years of existence. In relation with this intense activity, we have published four special issues and the present one is our fifth achievement. It collects papers submitted by the participants to the several events we have organized in the summer of 2019.

Umayahara and Nespolo present a historical perspective of the barely known pioneering work of Japanese crystallographers on modular structures, with a revised classification based on groupoid approach which generalizes the original description (article number 1900045). Nespolo and co-workers present a potentially case of a mis-attribution of X-ray diffraction data that could represent a trap for the less-experienced crystallographer (article number 1900063). Stoeger and Rotter discuss a complex case of polytypism and twinning in a crystal with simple chemistry and demonstrate how this sort of problems need a crystallographic knowledge well above what can be obtained in a normal training aiming at a routine approach (article number 1900164). Stoeger and co-workers present a different case of polytypism in a chemically more complex structure, where the coexistence of two different polytypes leads to residual peaks in the electron density (article number 1900182). Kurlin challenges the problem of quantifying the similarity between crystal structures, in search for an algorithm capable of discriminating nearly identical structures with



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different properties (article number 1900197). Last but not least, Svetogorov and co-workers provide a more experimental-related perspective on the new beamline at Kurchatov synchrotron radiation source to study, in particular, the real structure and the distribution of electron density in crystals (article number 1900184).

At the time of closing this editorial, I wish to express my gratitude to Wiley, for providing the opportunity to publish our fifth special issue, as well as to the Editor-in-Chief and the Managing Editor for their continuous support. MaThCryst is already projected towards further activities in the forthcoming weeks and I invite our readers to keep an eye on our schedule and our resources at www.crystallography.fr/mathcryst.

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DOI: 10.1002/crat.202000057