109. P. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M. B. Nardelli, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni, N. Colonna, I. Carnimeo, A. Dal Corso, S. De Gironcoli, P. Delugas, R. A. DiStasio, Jr., A. Ferretti, A. Floris, G. Fratesi, G. Fugallo, R. Gebauer, U. Gerstmann, F. Giustino, T. Gorni, J. Jia, M. Kawamura, H.-Y. Ko, A. Kokalj, E. KeÅekbenli, M. Lazzeri, M. Marsili, N. Marzari, F. Mauri, N. L. Nguyen, H.-V. Nguyen, A. Otero-de-la-Roza, L. Paulatto, S. Ponc8, D. Rocca, R. Sabatini, B. Santra, M. Schlipf, A. P. Seitsonen, A. Smogunov, I. Timrov, T. Thonhauser, P. Umari, N. Vast, X. Wu, S. Baroni, J. Phys. Condens. Matter, 2017, 29, 465901.

110. F. Furche, R. Ahlrichs, C. H-ttig, W. Klopper, M. Sierka, F. Weigend, WIREs Comput. Mol. Sci. 2014, 4, 91–100.

111. K. Schwarz in Selected Topics in Applications of Quantum Mechanics (Ed.: M. R. Pahlavani), InTech Open, London, 2015, 275–310.

112. P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka, J. Luitz, WIEN2k, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties, Tech. Univ. Wien, Vienna, 2001.

113. G. Kresse, J. Hafner, Phys. Rev. B 1993, 47, 558–561.

114. G. Kresse, J. Hafner, Phys. Rev. B 1994, 49, 14251–14269.

115. G. Kresse, J. Furthmeller, Comput. Mater. Sci. 1996, 6, 15–50.

116. G. Kresse, J. Furthmeller, Phys. Rev. B 1996, 54, 11169–11186.

Commission on Mathematical and Theoretical Crystallography

THE IUCr-MATHCRYST

was founded to promote and achieve the following aims:

- To strengthen links and interactions among crystallographers, mathematicians and theoretical physicists and chemists, and to promote a common language in these fields.
- To promote the presence at IUCr meetings of scientists working in the fields of mathematics, such as geometry, topology or functional analysis.
- To strengthen the recognition of crystallography as an interdisciplinary science in those fields where nowadays it is considered only to be a technique.
- To promote the publication of mathematical and theoretical papers in the journals of the Union.
- To encourage the development and dissemination of mathematical and theoretical methods, software and databases to solve crystallographic problems.
- To promote and organize symposia of interest to mathematical and theoretical crystallographers during IUCr congresses and meetings of regional associates, or in other scientific conferences possibly in cooperation with other Commissions of the Union
- To promote and organize meetings, workshops and schools possibly in collaboration with other Commissions particularly targeting post-graduate students and young scientists needing and willing to complete their education in crystallography.

Motivation

Far from having exhausted its research potential, Mathematical and Theoretical Crystallography (**MaThCryst**) face new challenges, not only in the very classical field of group theory (magnetic groups, chromatic groups, N-dimensional groups) and its applications (phase transitions, polymorphism and polytypism, twinning, bicrystallography, ferroic crystals), but also in several directions that previously were less strongly perceived as being directly related to crystallographic and crystal- chemical problems, such as graph theory, combinatorics, topology, number theory, discrete geometry, functional analysis, etc. The development of mathematical and theoretical crystallography will strengthen the interaction between crystallographers, mathematicians and materials scientists and will definitely contribute to the recognition of crystallography as an interdisciplinary science.

The outstanding success of applied crystallography in recent years has transformed common structural investigation into a routine task, often performed by researchers with no specific background in crystallography. Moreover, the success of automated structure solutions, whose results are persistently accepted without sufficient criticism, has contributed to the spread of the pernicious impression that a specific education in crystallography is no longer necessary in order to perform crystallographic tasks on a daily basis. The result is that nowadays crystallography is increasingly perceived as a technique, if not just as a tool, rather than an interdisciplinary science strongly interacting with fundamental and applied disciplines like mathematics, chemistry, physics, material science, geosciences and biosciences. As a consequence, the time devoted to crystallographic education in secondary, undergraduate and graduate courses is continuously shrinking, and the requirement of a solid background in crystallography is disappearing from the requirements of many positions that involve a considerable amount of crystallographic work.

The IUCr-MaThCryst commission was started on September 2002 as an informal working group from a nucleus of researchers who felt the necessity of trying to reverse the current trend towards “crystallography as a black-box tool”. From the didactic viewpoint, the commission aims at an activity which will hopefully cover the gap now existing between the “user” and the “specialist”. To achieve this, the commission regularly organizes summer schools and workshops and provides printed and printable (downloadable) material (do not hesitate to visit the commission’s website http://www.crystallography.fr/mathcryst/).