Keynote Lecture

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Making Crystals with a Purpose

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Since its inception in the late 80's, crystal engineering (CE), although intimately connected with crystallography, has represented an appealing alternative to the traditional work of experimental crystallographers. The prospect of exploiting the knowledge on intermolecular bonding in the bottom-up construction of crystals had led many structural chemists to abandon the (often frustrating) ancillary role of service crystallography to start making their own crystalline materials. At the same time, many synthetic chemists have found in CE new inspiration and new ideas for their synthetic skill and have moved from the preparation of molecules to that of new building blocks for supramolecular assemblies of higher complexity. There are several reasons for this (r)evolution: the success of supramolecular chemistry and the consequent shift of paradigm from molecule to molecular assembly, the need for new utilitarian objectives to research across the traditional subdivisions of chemistry, the extraordinary progress in computing and diffraction instrumentations, the need to increase control on crystal form selection (stable and metastable polymorphs, solvates etc.) and the consequences on biologically relevant solid state properties, etc. The net result has been not only a broadening of the field of solid state chemistry as a whole thanks to increased overlaps with materials chemistry, nanotechnology, and medicine, but also a new impulse, in a synergistic way, to crystallography, both in experimental methods and in computational modelling (structure from powder data, surface diffractometry, crystal structure prediction, etc.).
In this talk, some of these concepts will be illustrated from examples coming from our recent work at the University of Bologna. The bottom-up preparation of hybrid organic-organometallic crystals, mixed crystals, pharmaceutical and ionic co-crystals and photoreactive materials across the borders of organic, organometallic and metalorganic chemistry will be recounted with a focus on the relationship between size, shape, charge and functional group distribution over the building blocks and the structure and physico-chemical properties of the resulting crystalline materials.
[1] The future of structural chemistry nucleates in the present. D. Braga (2016) Israel J. Chem.
[2] Alloying barbituric and thiobarbituric acids: from solid solutions to a highly stable keto co-crystal form O. Shemchuk, D. Braga and F. Grepioni Chem. Commun., 2016, 52, 11815-11818
[3] Ionic Cocrystals of Racemic and Enantiopure Histidine: An Intriguing Case of Homochiral Preference D. Braga, L. Degli Esposti, K. Rubini, O. Shemchuk, and Fabrizia Grepioni Cryst. Growth Des., 2016, 16, 7263–7270.

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