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Molecular crystals

G. Gbabode[1*]

[1] Univ Rouen Normandie, Normandie Univ, SMS , UR 3233, F-76000 Rouen, France
*gabin.gbabode@univ-rouen.fr

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Molecular crystals are the basis of numerous advanced materials used nowadays in many field of applications such as pharmacy [1] (active pharmaceutical ingredients, excipients), electronics and opto-electronics (organic semiconductors) [2] or energy storage [3]. The properties of the materials are crucially dependent on the packing organization of the molecules in the crystalline state. Hence, the development of materials based on molecular crystals lie on a profound knowledge of their crystal arrangement and on the crystallization routes affording the desired crystal forms. In particular, polymorphism, which is defined as the ability of a compound to crystallize in more than one crystal structure, is a phenomenon which has to be understood and hopefully controlled. This lecture will, after a brief introduction on the practical interest of molecular crystals, review the fundamentals of crystallography, phase stability and crystallization that are needed to understand the challenge of designing molecular crystals. Then, a description of the main characterization techniques used to decipher the (often complex) phase behaviour of molecular compounds will be performed. Lastly, the author will select some case studies from his own research to highlight the wealth of crystal forms that even simple molecules can exhibit and the difficulties encountered to obtain one particular crystal form in certain cases.

[1] D. Braga, L. Casali, and F. Grepioni (2022): **The relevance of crystal forms in the pharmaceutical field: sword of Damocles or innovation tools?**, *Int. J. Mol. Sci.* 23, 9013-9041.

[2] C. Kunkel, J. T. Margraf, K. Chen, H. Oberhofer, and K. Reuter (2021): **Active discovery of organic semiconductors**, *Nature Communications* 12, 2422-2432.

[3] S. Horiuchi, S. Ishibashi, (2021): **Large polarization and record-high performance of energy storage induced by a phase change in organic molecular crystals**, *Chem. Sci.* 12, 14198-14206.

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☒ **Poster**

☐ **Oral**

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