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From molecules to materials, efficient crystal engineering of polar systems

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Technological progress enforces improved materials performance, therefore controlling synthesis of new systems requires moving from trial-and-error methods to comprehensive solutions. Understanding of molecular self-assembly requires assessment of all features which characterize building blocks and contribute to the unique physical properties of a crystal.
Novel polar materials designed for applications in linear or non-linear optics or as ferroelectrics have to fulfil several criteria concerning symmetry (necessary condition), electron properties of the building blocks as well as mechanical and optical stability. For this purpose the chosen components must possess high molecular polarizability/hyperpolarizability and what is more promote the formation of three dimensional noncentrosymmetric crystal structure.
Here we present our approach for efficient crystal engineering of multicomponent systems built of Active Pharmaceutical Ingredients (API) ensuring synthon formation flexibility and combined with push-pull molecules providing required electronic properties of a material [1]. The goal is to create a new polar material from the known starting components to ensure desired bulk properties of a crystal.
In our research we combine quantitative and in silico crystal engineering techniques together with prediction and measurements of optical properties. Noncovalent Interaction Analysis (NCI) [2], Hirshfeld surfaces and fingerprint plots [3], topology of electron density (ED) are a set of tools for the characterization of inter- and intramolecular interactions in the context of understanding structure-property relationship. This approach enables reliable assessment of selected co-formers as well as the obtained materials.
[1] Gryl, M., Acta Cryst., B71, (2015), 392.
[2] (a) Johnson, E. R., et al., J. Am. Chem. Soc. 132, (2010), 6498; (b) Contreras-Garcia, J., et al., J. Chem. Theory Comput., 7, (2011), 625.
[3] Spackman, M. A., Jayatilaka, D., CrystEngComm, 11, (2009), 19.
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