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Using electron density to understand cocrystal structures

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The formation of cocrystals ultimately depends on the compiting non-covalent interactions between molecular pairs A-A, B-B and A-B. However, the determination of these interactions is still nowadays a difficult issue for theoretical simulations.
We will present a simple method for the visualization of non-covalent interaction (known as NCI) based on the electron density and its derivatives [1]. It enables visualization ofrespulsive interactions, such as steric clashes; and attractive, such as hydrogen bonds, both fundamental for the understanding of molecular aggregation and cocrystal formation. It also reveals more subtle interactions, such as dispersive interactions, crucial for packing and stacking in pi-containing groups.
We will review the basics of the method and its application both to theoretical [2] and experimental (X-Ray derived) densities [3].
Finally, we will present an application on the stability of salicilic acid-based cocrystals, including both energetics and NCI analysis (see Figure 1).
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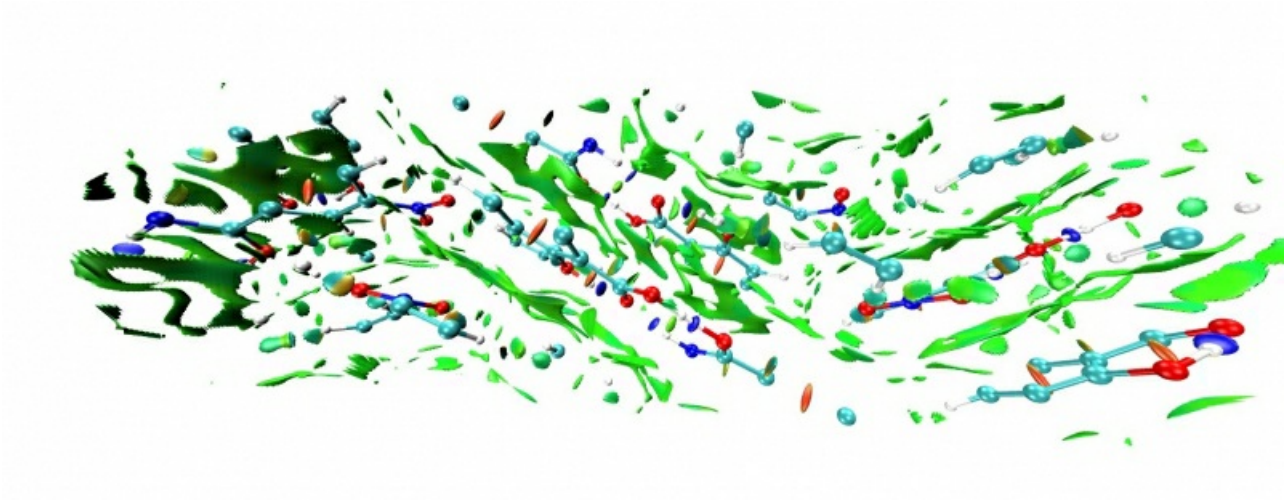

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