Poster Presentation

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Charge density studies of multicomponent crystals containing API - sulphanilamide

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Fast development of technology requires constant introduction of more and better solutions in material science. Efficient nonlinear optical smart materials have to fulfil several conditions including lack of inversion centre, high hyperpolarizabilities of the building blocks and mechanical stability [1]. Accomplishment of all of these nontrivial requirements is possible with multicomponent crystals. At least one of the building blocks increases electronic properties of material, while mutual assembly of building blocks provides non-centrosymmetricity. Promising components could be Active Pharmaceutical Ingredients (APIs) which possess synthon formation flexibility, are nontoxic and often cheap [2].
In our work sulphanilamide, an antibacterial drug, which is also a NLO chromophore was used as a starting point. The second component was chosen to utilize favourable donor\acceptors sites of sulphanilamide and to ensure polar mutual orientation of molecules. Crystal engineering techniques were combined with charge density studies in order to design materials with more efficient properties. Understanding of the intermolecular interactions and mutual assembly of building blocks in 3D structure is crucial for improving crystals performance. The properties of obtained materials were also predicted by theoretical calculations.
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