Putting Pressure on Multicomponent Crystals: Tuning Single-Crystal-to-Single-Crystal Transformations via Compositional Engineering

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Abstract

Tailoring the chemical composition through the design and synthesis of multicomponent crystals allows for the modification of crystalline solid properties via control over the intermolecular interaction landscape and aggregation preferences [1]. This can directly affect a crystal's response to external stimuli, such as high pressure, enabling access to single-crystal-to-single-crystal (SCSC) transformations not observed in the monocomponent crystals of pure coformers. In this context, the formation of multicomponent crystals can be presented as a relatively straightforward method for the synthesis of stimuli-responsive crystalline materials.

Among pressure-induced SCSC transformations reported for multicomponent crystals are phase transitions and solid-state reactions. Significant elastic deformations can also be regarded as continuous SCSC transformations if the crystallinity of the material is preserved. While physical changes observed upon compression provide insight into the effect of chemical diversification on phase stability and mechanical response, the research area concerning topochemical reactions is especially compelling. In these cases, not only does the molecular arrangement change, but the chemical nature of the components is altered. The aggregation of different chemical units within a crystal lattice allows for regio-selective reactions to take place [2] without the need for solvents, making such processes an environmentally friendly alternative to traditional synthesis [2]. Pressure is a powerful stimulus for inducing reactions in crystals [3], as lowering interatomic distances directly affects the energy barriers of chemical processes. It must be noted, however, that not all solid-state reactions are SCSC transformations, as they often lead to the loss of crystallinity or require additional stimuli like UV irradiation.

This presentation focuses on recent high-pressure investigations of multicomponent crystals, specifically highlighting observed SCSC transformations. These include phase transitions [4], cocrystals exhibiting significant negative linear compressibility over a wide range of pressure [5,6], and chemical reactions between coformers, such as proton transfer or the formation of new covalent bonds [4,7,8].

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References

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