Structural features of forming HOF and iHOF materials

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The highly ordered porous architectures attract wide interest owing to the broad range of functionalities such as catalytic properties, selective sorption and separation of chemicals, storage, charge-conductivity, and so on. Among the crystalline porous materials constructed through coordination bonds, covalent bonds, and hydrogen bonds, examples for the hydrogen bonded organic frameworks are still relatively rare. The long-range periodicity in HOF crystals is a product of the directionally specific short-range intermolecular interactions. We report the preparation and structures of two HOF families. One series is constructed by charge-assisted hydrogen bonds [1], while the other series is formed by hydrogen bonds without charge assistance [2] (Fig. 1).

We are performing a systematic study altering the electrostatic and steric properties of our framework constructing compounds. They are inspired by the Maruoka type chiral phase-transfer catalysts having potential application in catalysis, where porous architecture is an advantage. We show that porous materials can be tailored by designing the building block molecules, their functionality and flexibility, as well as by fine-tuning the supramolecular interactions among them. All these properties are in strong correlation with the molecular and crystal symmetries. Polymorphic and solvatomorphic forms of the frameworks themselves are also described. The presented work contributes to the systematic understanding of the structural features of the challenging formation of high porosity hydrogen bonded organic framework (HOF) and charged assisted hydrogen bonded organic framework (iHOF) materials.



Figure 1. Open pore hydrogen bond assisted organic framework having 29.8% void space in the unit cell.

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