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Engineering Molecular Crystals. James D. Wuest, Dépt. de Chimie, Univ. de Montréal, Montreal, Quebec, Canada.

No reliable method yet exists for predicting the detailed structure of molecular crystals, and the relationship between the structure of crystals and their physical properties remains poorly understood. For these reasons, attempts to engineer crystals for specific applications have remained largely empirical activities. However, important progress in this field is being made. One effective strategy in crystal engineering uses molecules that have been called *tectons*, which associate strongly according to well-established motifs. Tectons have arrays of sticky sites that direct association, linked to cores that orient the sticky sites and introduce other desirable molecular properties. In favorable cases, the oriented sticky sites play a dominant role in association and place each tecton in a predetermined position relative to its neighbors, leading to the programmed construction of particular molecular networks.

Normally, tectons cannot form structures that pack efficiently and simultaneously obey programmed directional interactions, so open networks are favored, with significant space for the inclusion of guests. Such materials are analogous to zeolites and related microporous inorganic materials. Many different sticky sites and cores can be used, giving molecular tectonics wide scope as a strategy for creating ordered materials with unique properties. In particular, we will describe hydrogen-bonded molecular crystals that 1) can be engineered with sub-nanometric precision; 2) use at least 75% of their volume to include guests, which can be exchanged without loss of crystallinity; 3) can be deformed by at least 30% without loss of crystallinity; and 4) react with external agents to give single crystals of new compounds with retention of the original crystalline architecture. We will also show how these materials can be characterized by a wide variety of physical methods, and we will highlight special properties of potential value in separation, catalysis, nanotechnology, and other areas.