

W0048

Engineering Crystal Architecture through Molecular Design: Applications of Supramolecular Assembly.

Michael D. Ward, Dept. of Chemical Engineering and Materials Science, Univ. of Minnesota.

Lamellar molecular host frameworks assembled by hydrogen-bonding between guanidinium ions and sulfonate moieties of organodisulfonate “pillars” contain well-defined pores with sizes, shapes and physicochemical characteristics can be tuned systematically through control of the pillar structure. These pores can be occupied by functional guest molecules, which serve as templates for the assembly of a number of compositionally identical framework isomers. These architecture and metrics of these frameworks are predictable, which has enabled *de novo* design of polar crystals for second harmonic generation, controlled organization of organic guest molecules in two-dimensional layers, and separation of isomeric organic compounds through batch crystallizations. The conformational flexibility of the guanidinium-sulfonate hydrogen-bonded sheet also allows the formation of porous hexagonal tubular architectures. Though the length scales differ by more than an order of magnitude, the lamellar-tubular isomerism is reminiscent of phase behavior observed for block copolymers and surfactant microstructures.