That composition and structure profoundly impact the properties of crystalline solids has provided impetus for exponential growth in the field of crystal engineering over the past 20 years. This lecture will address how crystal engineering has evolved from structure design (form) to control over bulk properties (function). Strategies for the generation of two classes of functional crystalline materials will be addressed:

Multicomponent pharmaceutical materials, MPMs, such as cocrystals have emerged as a fixture at the preformulation stage of drug development. This results from their modular and designable nature which facilitates the discovery of a wide range of new crystal forms of active pharmaceutical ingredients, APIs, with changed physicochemical properties. However, this does not mean that cocrystal discovery is yet routine. The concepts of “supramolecular heterosynthons” and “ionic cocrystals” will be explained as they pertain to the design of MPMs. We shall address the profound impact that cocrystallization can have upon solubility and bioavailability by presenting three case studies including one that addresses brain bioavailability of lithium.

Metal-Organic Materials (MOMs) that are built from metal or metal cluster “nodes” and organic “linkers” have captured the imagination of materials scientists because they are amenable to crystal engineering and they offer unprecedented levels of porosity. A family of MOMs, pillared grids, that afford exceptional control over composition, pore size and binding energy, will be detailed. Unprecedented selectivity for carbon capture in narrow pore MOMs will be highlighted.

In summary, this lecture will emphasize how the crystal engineering approach to materials design offers a paradigm shift from the more random, high-throughput methods that have traditionally been utilized in materials discovery and development with respect to pharmaceutical materials and porous materials. In short, how do we make the right material for the right application?

Figure. An ionic cocrystal involving a lithium salt and an amino acid.