1079-82-76 **Christopher E Wilmer*** (c.wilmer@gmail.com), 2145 Sheridan Rd. TECH E136, Evanston, IL 60208, and **Randall Q Snurr**, 2145 Sheridan Rd. TECH E136, Evanston, IL 60208. *Enumerating Chemically Detailed Crystals.*

In the last decade, a wealth of novel crystalline materials have been synthesized by what has come to be called "modular" or "reticular chemistry". This new approach, as opposed to serendipitous methods of the past, leverages the self-assembly of modular molecular "building blocks" that can only assemble in very specific orientations and allows one to design an enormous number of new crystals, far beyond what can actually be synthesized in a reasonable amount of time.

In this work, we present a novel approach of enumeratively generating all of the hypothetical crystals that can be made from a library of modular building blocks. The resulting crystals represent physical structures that can be screened in a high throughput manner via molecular simulations.

Using this method, we have generated 137,953 crystals and for each predicted a range of material properties using rapid computational simulations. In doing so, we illuminated hitherto unidentified structure-property relationships that could only have been recognized by taking a global view of the physical crystal space. (Received December 16, 2011)