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*Exploring frontiers of crystalline porous materials*

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We present a computational framework for the rapid identification and characterization of high surface area materials from within the vast chemical space of crystalline porous materials such as metal-organic frameworks (MOFs) or covalent organic frameworks (COFs). MOFs and COFs have been the subject of intense research interest due largely to their highly tunable structural properties and record-breaking internal surface areas; gravimetric surface area is one of the most addressed properties of porous materials, and has seen improvement by approximately a factor of twenty since the first reports. However, the design of MOFs with optimum chemical and geometrical properties remains a great challenge, due to the vast combinatorial space of building blocks and topologies in which they can be arranged. Efforts to identify high-performance materials have involved trial-and-error, observation-based design, computational enumeration and screening of large combinatorial libraries as well as optimization-based approaches. In our presentation, we will give an overview of techniques under development in our group, in particular, algorithms for 3D structure model assembly and material characterization. We will also present how these tools can be employed in both enumeration and optimization-based discovery of novel materials.