The self-assembly of building blocks ranging from molecules to colloidal nano-particles is an important tool for creating materials that address urgent challenges in energy conversion, gas storage, and catalysis. While the variety of building blocks that can be synthesized is ever expanding, our understanding of the formation mechanisms of nano-materials, and how these can be controlled experimentally, is still limited. Using molecular simulation and statistical mechanics, my group creates insight into the dynamics of self-assembly processes and develops strategies that guide the synthesis of new nano-materials. In this talk I will focus on our recent efforts to understand the nucleation and growth of porous framework materials.