Sipping from the Holy Grail: Molecular Modeling of the Formation of Ordered Nanoporous Materials

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Nanoporous materials such as zeolites and silica-based mesoporous materials are of great importance to many chemical industries because of their wide applications in catalysis and separations. The development of new applications in areas such as drug delivery, shape-selective sensors, and nano-electronics depends on tailoring material properties such as pore sizes, crystallite size and shape, and crystallite surface structures. The ability of synthetic materials chemists to tailor and target such properties is greatly hampered by our rather incomplete knowledge of mechanisms by which zeolites nucleate to form crystals. The atomic-level understanding of critical nucleation and the role of structure-directing agents (SDAs) remains quite poor because of the difficulties in characterizing the emergence of atomic-level order at the length scales of zeolite unit cells. In this talk, I discuss some of the modeling perspectives, methods, and results of my 15-year collaboration with Peter Monson of the UMass Amherst Chemical Engineering Department, which have shed new light on the physical chemistry of silica polymerization and zeolite formation.

We view zeolite formation as a 3D network formation problem resulting from the fluctuating connectivities between silica species in solution. We have developed (discrete-space) lattice models and (continuum space) off-lattice models based on the near degeneracy of silica lattice energies. Sampling fluctuating network connectivities in 3D space is a notoriously complex computational problem, which we have addressed with a variety of Monte Carlo simulation algorithms. In this talk, I will share essential aspects of our Monte Carlo procedures, and will discuss results on silica polymerization, zeolite crystallization, and mesopore formation.