NIRT- An Interdisciplinary Approach to Understanding the Growth of Nanoporous Materials

P. A. Monson, S. M. Auerbach, M. Tsapatsis - University of Massachusetts
D. G. Vlachos, R. Lobo - University of Delaware

NSF-CTS-0103010

Background:

- The ability to fabricate complex, nanostructured materials tailored for specialized applications remains an elusive goal of the National Nanotechnology Initiative.

- An exciting strategy for such materials synthesis involves hierarchical assembly of supramolecular precursors, to form complex organic-inorganic structures with long-range order. This leads to nanoporous solids with applications ranging from catalysis to separations to optical-electronics to bioimplants.

- Need a fundamental understanding of the structures and mechanisms that control hierarchical assembly.

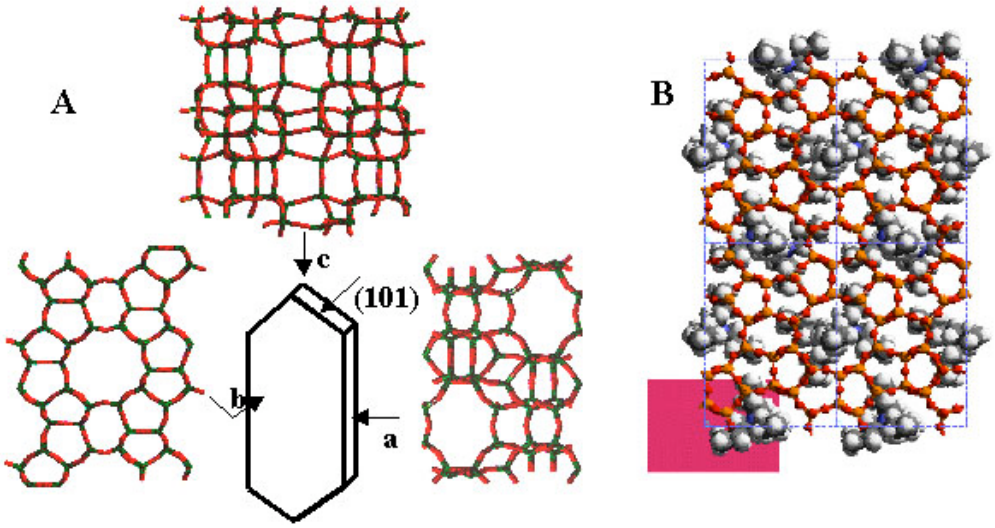

Figure 1. A: Schematic of the MFI framework along different crystallographic directions; and B: Schematic of TPA location in the MFI framework.

- This NIRT project combines research in experimental synthesis and characterization of silicalite (MFI) with atomistic and multiscale modeling to develop this understanding.

Results:

• There is a pronounced effect on MFI crystal growth kinetics and MFI crystal habit when the synthesis is performed with the dimer and trimer of TPA.

• Our work on the imaging of subcolloidal particles does not indicate the presence of defined nanoslabs as has been recently proposed in the literature.

• A base case molecular model of silica is capable of forming mechanically stable solid structures that are similar to those of real silica. This model will be used in studies of silicalite-1 structure and formation.

• The NMR spectrum depends on zeolite particle size (see figure 2).

Scientific Uniqueness:

• As a team, the investigators bring a powerful perspective and established collaborations to bear on a major problem in materials science and engineering.

• Experiments – Kokkoli, Lobo, Sherman and Tsapatsis. Expertise in synthesis and characterization. Collaboration with Toby at NIST adds expertise for studying disordered structures.

• Theory – Auerbach, Monson, Muthukumar and Vlachos. Wide-ranging experience in statistical mechanical and multiscale modeling and simulation of complex materials.

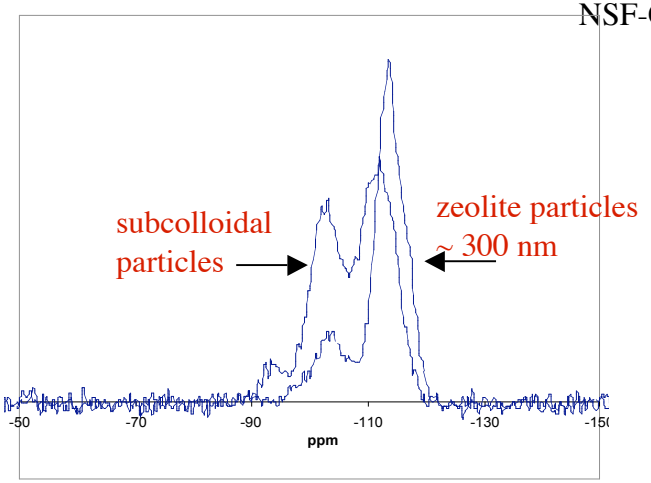

Figure 2. ^{29}Si MAS NMR of silicalite-1 subcolloidal particles and 300 nm zeolite particles.

Impact:

• The ability to manipulate the interactions between nanoparticles at the heart of the problem of synthesis of complex materials with well-defined structure at several length scales.

• The project investigates a case of self-assembly that is typical of the nanoscale regime.

• On the basis of this research, researchers will be able to tackle similar problems within a tested and organized framework.

• Framework for teaching the detailed experimental and theoretical research methods as well as the organizing principles under which to approach research in this field.