

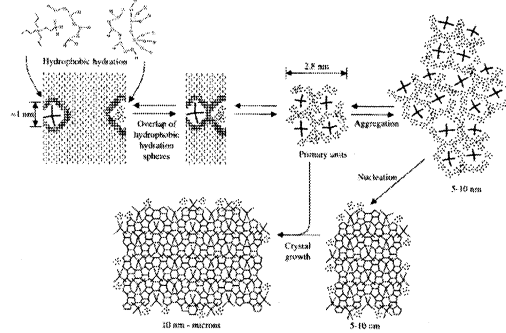
Quantitative Approaches to Templated-Mediated Nucleation
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Synthesis of new materials in solution typically requires both nucleation and growth.

For many templated materials, nucleation is still not understood.

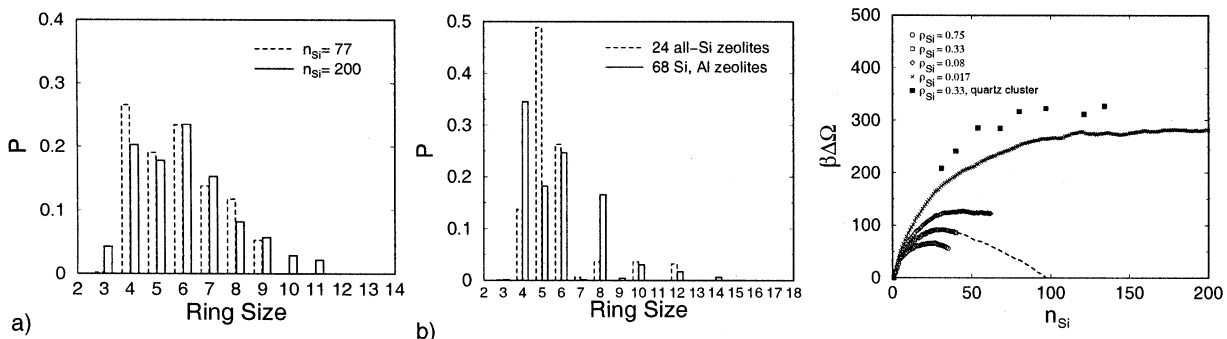
Length scale bigger than NMR and smaller than scattering.

For example, the nucleation mechanism of zeolites is unresolved. Perhaps:



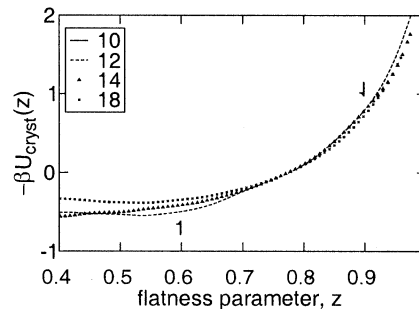
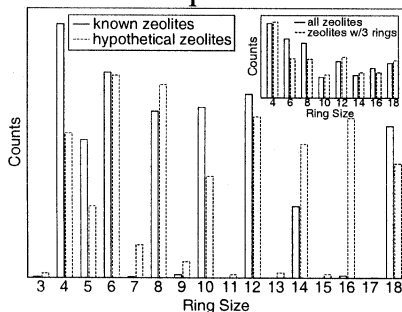
M. E. Davis, 1999.

Simulation approach is non-trivial. Silica system is glassy and slow to equilibrate. Need reactive force field. Need powerful Monte Carlo moves. Nucleated clusters are different from crystal:



Ring size distribution has odd-membered rings—zeolites do not. Free energy of amorphous cluster is lower than that of a small zeolite crystal (Wu and Deem, 2002). Is this also true for clusters in the presence of template? We do not know yet.

Some other questions:



Why no 16-ring zeolites? Ring flattening energy ~ zeolite/template interaction
 Ring flattening energy also ~zeolite destabilization energy (Curtis and Deem, 2003).

Combinatorial Chemistry (HTE)

M.W. Deem

- How best to search variable space?
 - Composition, T, P, pH, processing variables, ...
 - Three-dimensional spatial arrangement
 - Protein sequence - Evolution
 - Biocatalysis, sensors, drugs, assays
- Grid search, point mutation, recombination
 - The curse of dimensionality
- How to make use of known information?
 - Theory, database information
 - Chemical intuition, prior experiments
- The Monte Carlo paradigm
 - Searching variable space
 - \cong Searching configuration space
 - Incorporation of *a priori* information
 - \cong Biased Monte Carlo
 - Improvements of 10^6 shown
 - SYMYX library design group (= Deem people)
- Parallels to nature
 - The immune system
 - Evolution of antibody genes (4×10^8 years)
 - Regulation of gene expression (10 - 10^4 years?)
 - Adaptation of antibodies to particular antigen/disease (10 days – 30 years)