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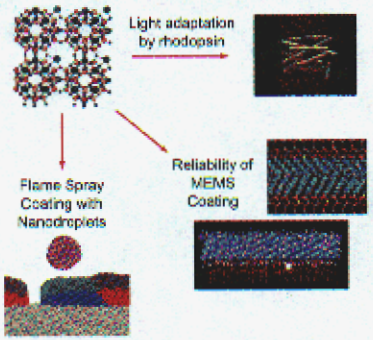
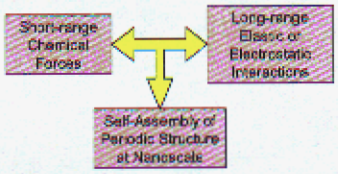
Nanoscale Theory and Simulation

Eliot Fang, Corbett Battaile, Mike Chandross, Paul Crozier, Liz Holm, Gary Kellogg, Mark Stevens, Frank van Swol, and Ed Webb

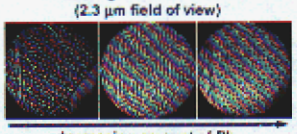
Quantum & Atomistic Approaches



Self-assembly can be used to create templates for nanostructure fabrication



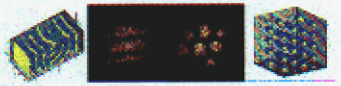
LEEM Images of Pb/Cu at 673 K (2.3 μm field of view)



Increasing amount of Pb

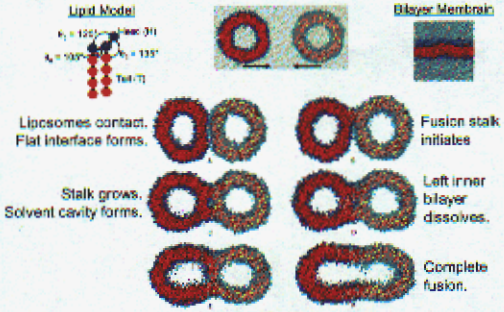
Droplet size distribution peaked at 67 ± 8 nm

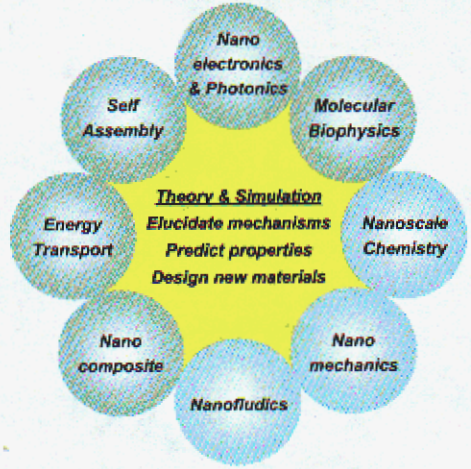
Modeling and simulation of self-assembly provide the scientific underpinnings for technological advances.



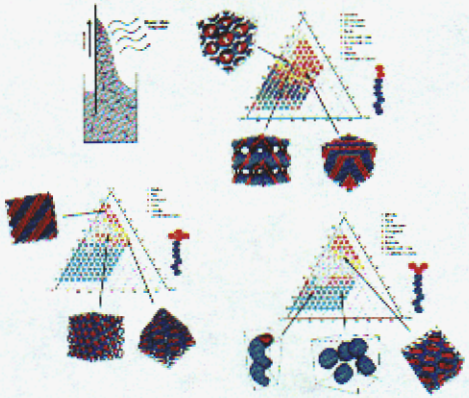
- Science – identify fundamental parameters (boundary energy and stress mismatch) that lead to self-assembly and pattern formation
- Technology - Learn how to control properties (pattern type, feature size, long-range order, etc.)

Simulation of Membrane Fusion using Coarse-Grain Model





Predict evaporation-induced self-assembly during dip-coating

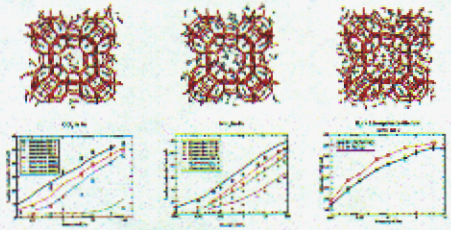


To understand the mechanism of biomembrane fusion mechanism is essential to biology and technology developments.

- Vesicular trafficking
- Fertilization
- Viral infection
- Liposome based drug delivery
- Biosensor development
- Nanotransport

Chemistry and Adsorption of Small Molecules in the Nanopores inside LTA Zeolites

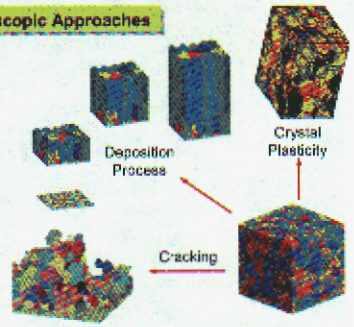
Desiccant capacity is found to degrade after several years of use, and proposed explanation is reaction of ammonia, carbon dioxide and water in the nanopores inside the zeolite.



Modeling local chemistry in the presence of collective phenomena is a critical step toward scientific understanding of complex nanoporous materials.

- Gibbs Ensemble Monte Carlo simulations were performed to determine equilibrium loadings.
- Quantum mechanics calculations are running to calculate the energetics of the reaction.

Mesoscopic Approaches



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