# Nanoscale Science and Engineering Center for Directed Assembly of Nanostructures

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The mission of the center is to integrate research, education, and technology dissemination, and serve as a national resource for fundamental knowledge and applications, in directed assembly of nanostructures. The center will: 1. Combine computational design with experimentation to discover novel pathways to assemble functional multiscale nanostructures with junctions and interfaces between structurally, dimensionally, and compositionally different nanoscale building blocks. 2. Excite and educate a diverse cadre of students of all ages from K-12 through postdoctorate in nanoscale science and engineering. 3. Work hand-in-hand with industry to develop nanotechnology for the benefit of society. (1)

NSEC research on directed assembly of nanostructures involves two major areas of emphasis: "Nanoparticle Gels and Polymer Nanocomposites" and "Nanostructured Biomolecule Composite Architectures." Each thrust group is supported by multiscale theory and modeling, as well as extensive characterization efforts. The Center also includes an insightful research component, "Socioeconomic Implications of Nanotechnology," which involves considering strategies for managing radical innovations in this exciting new program of study.

**Nanoparticle Gels and Polymer Nanocomposites** (2)
The research aims of the Nanoparticle Gels and Polymer Nanocomposites Thrust are three-fold: (1) fundamental studies of the synthesis, phase behavior, and structure of chemically heterogeneous nanoparticles, (2) development of directed assembly routes for producing 3D nanostructured materials, and (3) development and characterization of novel polymer nanocomposites. Key initial developments include the synthesis of monodisperse, gold and silica nanoparticles, with diameters in the 3-15 nm range, surface functionalized with primary amine, carboxyl, PDMS, or aliphatic groups. These inorganic nanoparticles will be used in the directed assembly of 3D structures and biomolecular materials. New synthetic pathways to foldamers and heterostructured polymer nanoparticles are also being developed; these molecules, which adopt ordered conformations, are useful as nanoscale building blocks. Fundamental folding studies are underway and comparisons with biological nucleation-elongation polymerization are being made to assess the opportunity to generate synthetic coherent motion at the nanoscale. Phase behavior and the structure of nanoscale building blocks are being studied by a range of techniques, including light scattering, microscopy, and complemented by statistical mechanics.

**Nanostructured Biomolecule Composite Architectures** (3)
The Nanostructured Biomolecule Composite Architectures Thrust conducts research into how life's basic building blocks can be incorporated into artificial nanomaterials to build devices that could one day diagnose illness and materials that could repair damaged human tissue. Its research focuses on the preparation, characterization, and application of biomolecule/nanoparticle composite materials that provide for structure and function. This enables specific applications ranging from *in situ* nanoparticle functionalization to tissue engineering to catalyst arrays. Substantial progress has been made in generating functional

nanocomposites that contain biocatalytic activity. Enzymes have been attached to two types of nanostructures: water-solubilized carbon nanotubes and silicon nanopillars. In addition, protein-DNA complexes have been developed as a precursor of biological nanostructures. Biomolecular interactions are exquisitely selective, and offer the promise of allowing unique structures with important functions to be designed and synthesized. We have focused on two types of biological nanoarchitectures: protein-DNA nanomolecular assemblies for use as highly sensitive sensor elements and protein-DNA-lipid composites.

**Multiscale Theory and Modeling** (4)
The Multiscale Theory and Modeling team offers expertise in electronic structure calculations, atomistic and coarse-grained molecular dynamics, and Monte Carlo simulations, as well as in statistical mechanical theoretical methods. Using their interdisciplinary expertise, members are creating the needed scientific base to enable design and directed assembly of a wide range of nanostructures. Such design will be based on multiscale models under development that employ systematic coarse graining procedures to incorporate electronic and molecular level effects into larger scale models. These larger scale models will be capable of predicting properties and functionality at experimental length and time scales. These models also will be used to understand and design thermodynamically and kinetically based paths towards assembly of desired nanoarchitectures. Such design will involve exploration of novel avenues to create surface assembly sites on nanoscale building blocks, so that their assembly in imposed force fields can be directed to enable the synthesis of functional nanoscale architectures for device and systems applications.

**Socioeconomic Implications of Nanotechnology** (5)
In addition to its multidisciplinary materials science and engineering research components, the Center for Directed Assembly of Nanostructures includes an innovative research module that does not involve high tech laboratory experiments. In the "Socioeconomic Implications of Nanotechnology" research component, results from social and ethical issues studies will be equally as critical as the scientific discoveries to the future of this emerging field. Rensselaer Polytechnic Institute's Lally School of Management has established a team of researchers to consider strategies for managing the many radical innovations of nanotechnology. Members have begun by studying how nanotechnology compares with other megatrends such as biotechnology, MEMS (microelectromechanical systems), and superconductors, in its effects on required core competencies, training, and education. Researchers have compiled a database of 140 nanotechnology companies, and have begun to develop a set of questions to use with scientists and engineers in the nanotechnology field to understand what drives their research agenda, what triggers their interest in nanotechnology, and what their views are about future applications and impacts. Team members also have developed a preliminary protocol that they have tested on company representatives from large established firms. Their objective is to understand how organizations came to invest in nanotechnology and what impact those investments have had to date.

**Educational Outreach** (6)
The first year Educational Outreach program focused on:

A. The summer outreach program to our 5 undergraduate partner institutions (Morehouse, Mt. Holyoke, Smith, Spelman, and Williams Colleges).

B. The collaboration with the Troy Junior Museum to use a planetarium setting to teach children about the molecular scale world.
C. Outreach to High School Teachers
D. Investment in the BOAST program at UIUC

**A. Summer Outreach to Undergraduate Partners:** Nine undergraduates from our partner institutions came to RPI this summer and worked in nanotechnology. The projects they developed are being continued at their host institution and will continue next summer as well. Six of 8 faculty involved in the program have traveled to Rensselaer and faculty from RPI have traveled to 3 of the 5 partner schools.

**B. Troy Junior Museum Project:** Our Molecularium project uses a planetarium to take students (K-3) to the molecular level (instead of space) to teach them about the nanoscale. Our pilot program (7 minutes) is complete and hands on activities before and after the molecularium show have been developed. Three pilot schools have been through the program to date. We will have a grand opening on December 11, 2002. Full evaluation of the program will begin in the Spring of 2003. As one parent said, "My 4 year old daughter got up the next morning and said, "Mommy, my juice is made of molecules, but you can't SEE them!"

**C. Outreach to High Schools:** Two teachers and 2 students from Schalmont High School, Rotterdam NY, spent 6 weeks at RPI learning about nanotechnology and developing 2 multimedia modules that will be used in the Environmental Science and Biology courses in the 2002/2003 school year. If successful, they will be exported to other schools.

**D. BOAST:** Engineering faculty and graduate and undergraduate members of the Nanoscale Science and Engineering Center team at University of Illinois at Urbana-Champaign (UIUC) have become involved in an active science education program for academically at-risk youngsters called Bouchet Outreach and Achievement in Science and Technology (BOAST). The mission of BOAST is to stimulate children's interest in science and to provide a national resource for hands-on science and Internet lessons. The program serves kindergarten through fifth grade students who spend about two and a half hours after school each day focusing on homework and educational activities, including field trips, hands-on science lessons, and Internet workshops.

(1) For more information about the NSEC for Directed Assembly of Nanostructures, link to http://www.rpi.edu/dept/nsec/
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