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. NSEC research on directed assembly of nanostructures involves two major areas of emphasis: "Nanoparticle Gels and Polymer Nano-composites" and "Nanostructured Biomolecule Composite Architectures." Each thrust group is supported by multiscale theory and modeling and extensive characterization efforts. The Center also includes insightful research into "Socioeconomic Implications of Nanotechnology," which involves considering strategies for managing radical innovations in this important new area. (1)

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 developments include the synthesis of chemically heterogeneous gold and silica nanoparticles as well as gold nanoclusters and nanowires. These nanoscale building blocks will be used in the directed assembly of 3-D structures, as novel fillers in polymer nanocomposites, and in the assembly of biomolecular materials. New synthetic pathways to foldamers and heterostructured polymer nanoparticles are also being developed. These molecules, which adopt ordered conformations, are useful as model nanoscale building blocks. The phase behavior, structure, and assembly of these building blocks is being studied by a range of experimental techniques, including scattering and rheological measurements, and complemented by statistical mechanical theory. A qualitatively new dependence of the fluid-fluid phase boundaries on polymer-particle size asymmetry was discovered, with excellent agreement obtained between the no-adjustable-parameter theory and experiment. Nanoparticle gel-based inks have been developed for the directed assembly of 3-D periodic structures. The effects of nanoparticle and nanotube fillers on the structure and properties of polymer composites have been studied. We have produced polymer nanocomposites with a six-fold enhancement in their strain-to-failure relative to the pure polymer matrix. We have also initiated the development of a microscopic theory of the equilibrium properties of model polymer-particle mixtures under the dense polymer conditions relevant to polymer nanocomposites.

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 diagnose illness and materials that could repair damaged human tissue. Its research focuses on the preparation, characterization, and application of biomolecule containing composite materials that provide for structure and function that will enable specific applications ranging from *in situ* nanoparticle functionalization to tissue engineering to catalyst arrays. Key developments include protein attachment to carbon nanotubes that has yielded nanocomposites with high enzymatic activity, including those with high solubility in aqueous solutions. Also, nanoparticles have been generated using cationic emulsion polymerization. These platforms can be easily manipulated to yield biological functions with important applications, ranging from antifouling surfaces for industrial and biomedical use, and countermeasures against chemical and biological warfare. Computational techniques have provided a critical level of fundamental understanding of the physicochemical determinants of a protein's nano-environment that renders it functional, especially in non-biological environments. Nanomolecular assemblies based on biological molecules, as well as small molecule natural products, have also been developed. Cationic membrane lipids and DNA have been self-assembled into nanoporous lamellar structures, in which a 1-D DNA lattice is intercalated between planar lipid membranes to provide controlled inter-DNA spacing, thereby enabling templated synthesis of inorganic nanostructured catalytic materials and semiconductors. High-axial-ratio nanostructures formed by hierarchical self-assembly of alkylphenol glycosides found in a variety of plants have been prepared to form nanoscale helical/tubular nano-architectures with diameters of 50-100 nm and lengths of >1 mm.

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. Research on multiscale simulation methods has resulted in a novel Empirical Potential Interaction Coarsening (EPIC) method that constructs effective pair potentials between coarse-grained polymer segments that retain atomistic scale information and results in major savings in computational time. The simulations were shown to yield conformational statistics consistent with molecular-level simulations and extend the size of polyethylene melts that can be treated to molecular weights greater than 100,000 g/mol. These larger scale models will be capable of predicting properties and functionality at experimental length and time scales and will also 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 this NSEC research component, results from social and ethical issues studies will be placed on a similar footing with the scientific discoveries in establishing the future of this emerging field. Rensselaer Polytechnic Institute's Lally School of Management and Technology 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 in its effects on required core competencies, training, and education. Researchers have compiled a database of 140 nanotechnology companies, and have developed a set of

questions that have been used 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 have also developed a protocol that they have used with company representatives from large established firms. They are beginning to understand how organizations came to invest in nanotechnology and the impact such investments are having.

Educational Outreach (6)
The NSEC's active Educational Outreach program is focused on:

A. Summer Outreach to Undergraduate Partners: Undergraduates from our partner colleges (Morehouse, Mt. Holyoke, Smith, Spelman, and Williams Colleges) came to RPI again this summer and actively worked in nanotechnology research. The projects they developed are continued at their host institution during the academic year and will continue at RPI over next summer as well. College faculty involved in the program traveled to Rensselaer and RPI faculty traveled to the partner colleges to ensure collaboration.

B. Troy Junior Museum Project: Our "molecularium" project uses a planetarium setting to take students (K-3) to the molecular level (instead of space) to teach them about the nanoscale. Our pilot molecularium program (7 minutes) was completed and hands-on activities before and after the show were developed. Three pilot schools have been through the program and a grand opening was held on December 11, 2002. Careful evaluation of the program led to a proposal to the NSF for the production of two full-length professional shows in the coming three years.

C. Outreach to High Schools: A successful program in Summer 2002 with 2 teachers and 2 students from Schalmont High School, Rotterdam NY, in which they spent 6 weeks at RPI learning about nanotechnology and developing 2 multimedia modules that were used in their environmental science and biology courses in the 2002/2003 school year, was extended at RPI in Summer 2003 to teachers and students from three additional schools in New York State, Croton-Harmon and Ballston Spa high schools and Albany Academy.

D. BOAST: Engineering faculty and graduate and undergraduate members of the NSEC team at the University of Illinois at Urbana-Champaign (UIUC) continued their active involvement in an exciting science education program for academically at-risk youngsters called Bouchet Outreach and Achievement in Science and Technology (BOAST). The successful 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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