The Center for Biological and Environmental Nanotechnology (CBEN)

Annual Report to the National Science Foundation (NSF)

Report Year: 2001
## Table of Contents

2. Executive Summary .................................................................................................................... 1  
3. Quantifiable Outputs .................................................................................................................. 4  
4. Mission and Broader Impact ...................................................................................................... 5  
5. Research Accomplishments and Plans ........................................................................................ 7  
   5.1 Theme 1: Nanoscience at the Wet/Dry Interface ................................................................. 7  
      5.1.1 Biological activity of bio-nanoconjugates .................................................................. 7  
      5.1.2 Single-walled carbon nanotubes in complex aqueous media ............................... 9  
      5.1.3 Spectroscopic studies on carbon nanomaterials .................................................... 10  
      5.1.4 Protein Nanowires ................................................................................................. 11  
   5.2 Theme 2: Nanomaterials in Bioengineering ................................................................. 13  
      5.2.1 Metal nanoshells in bioengineering ...................................................................... 13  
      5.2.2 Nanocomposites for bone replacement .................................................................... 16  
   5.3 Theme 3: The Environmental Implications of Nanotechnology .................................. 20  
      5.3.1 Nanostructured membranes and their applications ........................................... 20  
      5.3.2 Fluid flow on the nanoscale .................................................................................... 22  
      5.3.3 Nanomaterial fate and transport in the environment .......................................... 23  
   5.4 Theme 4: Nanomanufacturing Facility .......................................................................... 26  
6. Education and Human Resources .......................................................................................... 29  
   6.1 K-12 Programs ................................................................................................................... 29  
      6.1.1 CHEM 570, Spring Content Course ..................................................................... 30  
      6.1.2 Summer Internship ................................................................................................. 31  
      6.1.3 Model Science Lab II .............................................................................................. 31  
      6.1.4 Laredo/Rice IPC Teacher Training Workshop ....................................................... 32  
      6.1.5 High-School Summer Academy ............................................................................ 32  
      6.1.6 Nanokids™ Curriculum Development .................................................................. 32  
      6.1.7 Other Activities ....................................................................................................... 33  
   6.2 Undergraduate Programs .................................................................................................. 34  
      6.2.1 MREU Program ...................................................................................................... 34  
      6.2.2 New Undergraduate Courses under Development .............................................. 35  
      6.2.3 Undergraduate Courses Modified .......................................................................... 35  
   6.3 Graduate Programs ......................................................................................................... 35  
      6.3.1 New Graduate Courses under Development ....................................................... 36  
      6.3.2 Entrepreneurship Education .................................................................................. 36  
      6.3.3 Graduate Courses Modified .................................................................................. 37  
      6.3.4 Hochschule Bremerhaven University of Applied Sciences .................................. 38  
   6.4 Community Programs ..................................................................................................... 38  
   6.5 Diversity .......................................................................................................................... 38  
7. Outreach and Knowledge Transfer ....................................................................................... 40  
   7.1 Nanotechnology and Environment Workshop ............................................................ 40  
   7.2 Annual Conference ......................................................................................................... 40  
   7.3 Industrial Affiliates Program ......................................................................................... 40  
   7.4 Industrial Collaborations/Interactions .......................................................................... 41  
   7.5 Entrepreneurship ............................................................................................................. 41  
   7.6 Presentations/Other Outreach ....................................................................................... 41
2. Executive Summary

Nanomaterials have the potential to influence nearly all aspects of our society bringing profound benefits for human health and our environment. To realize this potential, however, nanotechnology will need to undergo a smooth transformation from a young, promising discipline into an established commercial enterprise. We believe the role of a nanoscience and engineering center is to facilitate this growth in whatever way is appropriate for its members. In our center, we specialize in the application of nanomaterials to biological and environmental engineering; many examples from our center’s research illustrate that technologies which arise from the interface between manmade nanostructures and biological systems can be extraordinarily powerful. Research alone does not address the growing pains of this field, and our center also supports outreach efforts designed to sustain this rapid changing area. Programs aim to create a core nanotechnology curriculum, to develop trained nanoscientists, and to ensure early nanotechnologies are translated into tangible success stories. All of these activities support our mission, which is to create sustainable nanotechnologies that improve human health and the environment.

The specific programs in our center were constructed as tightly integrated research, outreach, and dissemination efforts focused in biological and environmental engineering. Fundamental studies of the connection between nanomaterials and biology, what we term the wet/dry interface, are the core research of this center (Theme 1). It is only with a deep understanding of this interface that nanobiotechnology and nanoenvironmental technology can be invented and optimized. We also support interdisciplinary research that blends nanochemistry with environmental and bioengineering, with the goals of exploring and developing new ways of using nanotechnology (Themes 2,3,4). Our knowledge transfer activities are designed to guide early technologies which result from this research into the commercial sector. An important feature of our approach is the recognition of the increasingly important role that academic inventors play in technology transfer. Finally, we sponsor educational programs that develop teachers, students, and citizens who are well informed and enthusiastic about nanotechnology. We have included a wide range of campus partners to help in these endeavors, including the Jones Graduate School of Management and the Center for Education. Together with the research efforts we provide the necessary breadth for bringing nanoscience to the academic community and the public at large.

Cross-Cutting Research: Nanosystems at the Interface with Living Systems

Nature provides us with breathtaking examples of elegant and functional nanosystems. From magnetic bacteria that sense the earth’s magnetic field using nanosized bar magnets, to the nanoparticle-mediated transport of inorganic material in wastewater, the world around us is replete with examples of nanomaterials in action. These examples illustrate that the interaction between nanosystems and biosystems can be a strong and important one, a lesson that nanoscientists are only beginning to explore in the design of artificial, chemically prepared nano-biosystems. Our center’s research seeks to understand and ultimately manipulate this interaction as it manifests over a wide range of length scales, from enzymes to the earth’s environment.

The study of this problem requires an interlocking set of collaborative programs that examine the issue over these length scales, which are inexorably linked in living systems. Center projects in theme #1 progress in their study of bio-nano interactions from basic solution phase behavior, to
biochemical processes, and ultimately to cellular interactions. Theme #2 builds on this knowledge base to use nano-biosystems as tools to solve problems in bioengineering. Some projects in theme #3 develop a large-scale view of how artificial nanostructures will interact with the environment, while others exploit state-of-the-art nanochemistry to construct materials useful in environmental remediation, resource recovery, and industrial separations.

These three overlapping yet distinct theme areas have multiple connection points. For example, researchers in Theme #1 will collaborate with researchers in Themes #2 and #3 to tailor new varieties of nanomaterials for desired applications. Work on solvation properties of nanoparticles (Theme #1) will be complemented by work on nanoparticle surface chemistry, aggregation, and contaminant adsorption in aqueous environments (Theme #3). Nanobiosystems developed in Themes #1 and 2 may find application in environmental measurements (Theme #3). Methods for fabricating new nanostructured membranes designed for environmental applications (Theme #3) will also find application in our nanomaterials production facility (Theme #4).

Rethinking Industrial Outreach: Innovative Programs to Nurture Commercialization

Many of our center’s members have had direct involvement with the commercialization of their research ideas, in particular those based on nanomaterials. We have taken the lessons learned from their experience and developed an innovative set of center programs designed to create effective academic-industrial collaborations. We include outreach to small and startup companies because of their increasing importance in high technology development. To provide center members with the skills needed for the more active interactions such organizations demand, we are partnering with the Rice’s Jones Graduate School of Management to establish an entrepreneurial education program. These activities bring scientists, students and business experts together to ensure the formation of successful startups based on our center’s research. We are also developing a concrete strategy for handling the challenging issues associated with nanomaterial scaleup (Theme #4). Even limited applications testing of a nanosystem under realistic conditions can require larger quantities of material. Such scaleup is often beyond the scope of an academic lab, yet established companies are unwilling to invest in making large quantities without sufficient testing in-hand. Our nanomaterials production facility provides a solution to this problem. Directed by both chemists and chemical engineers, it will take on scale-up projects which address the practical production of materials.

A Focus on Teachers: Shaping the mentor’s of tomorrow’s diverse young scientists

While we sponsor a broad array of educational activities, our central belief is that the best investment we can make in the nanoscience and engineering workforce of the future is the development of a cadre of talented educators able to inspire students from the 9th grade level onwards. Our centerpiece program in teacher training targets this goal. We are using our center’s
resources to provide content lectures and tutoring to educators, to offer them a meaningful experience in our research laboratories, and to provide them a sabbatical semester to focus on integrating these experiences into their teaching style. Our relationships with these teachers continue as we welcome into the center students they identify for programs designed to support them as their career plans develop. The diverse nature of the Houston school district, from which we will draw our high school participants, allows us to support minority science students throughout their formative educational years. Our commitment to educators continues in programs designed for graduate students, many of whom will go onto positions as educators.

Rice University: The Early Leader in Nanoscience and Engineering

While it is difficult to pinpoint an exact birthplace of nanoscience, Rice University would certainly be a contender in any debate. Since the discovery of C$_{60}$ in 1984 through the present, this institution has shown a commitment to this interdisciplinary area. The university established in 1995 the Center for Nanoscale Science and Technology (CNST) to provide focus to its fundraising activities, as well as to serve as an umbrella organization for the many new nanoscience and engineering hires. Unlike a federally funded center such as a NSEC, this entity does not support research per-se, but instead acts as a conduit for institutional matching, building and equipment funds. A new building, Dell Butcher Hall (see right), was commissioned to act as the headquarters for nano-related research. This long-term commitment to nanoscience, focused principally in the area of chemically prepared nanostructures, has resulted in a base of both people and facilities unparalleled in the country.

Transforming Nanoscience and Engineering at Rice

While our center’s vision is to transform nanoscience and technology into a global discipline, this NSEC is also transforming our institution. Though our center’s members all have a strong track record in collaborative and interdisciplinary research, the proposed projects are not small extensions of these successful efforts. Rather they are new directions that were shaped by the overarching research mission of understanding and manipulating the interface between nanosystems and the living world. In this way, many research programs at Rice have altered course to converge on the center mission. We have used the center’s existence to lobby for a new approach to shared equipment maintenance across campus. Now under the control of a faculty group, joint instrumentation can now be used by a wider range of faculty for less total cost. The center also serves as a catalyst for developing innovative outreach strategies based on Rice’s decade-long experience with communicating and transferring nanoscience to the surrounding communities. Societal implications of this emerging discipline are being explored in collaboration with distinguished scholars in Rice’s James Baker III Institute for Public Policy. Our emphasis on the transformation of this young and exciting area of research has the added benefit of transforming our institution, and promises to leave a lasting effect on both the academic and larger worlds.
3. Quantifiable Outputs

<table>
<thead>
<tr>
<th>Outputs</th>
<th>Reporting Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>Publications resulted from NSEC Support</td>
<td></td>
</tr>
<tr>
<td>in Peer Reviewed Technical Journals</td>
<td>7, 5, 5*</td>
</tr>
<tr>
<td>in Peer Reviewed Conference Proceedings</td>
<td>0</td>
</tr>
<tr>
<td>in Trade Journals</td>
<td>1</td>
</tr>
<tr>
<td>with Multiple Authors</td>
<td>6, 5, 5*</td>
</tr>
<tr>
<td>co-authored with NSEC faculty</td>
<td>2, 2, 1*</td>
</tr>
<tr>
<td>NSEC Technology Transfer</td>
<td></td>
</tr>
<tr>
<td>Inventions Disclosed</td>
<td>1</td>
</tr>
<tr>
<td>Patents Filed</td>
<td>1</td>
</tr>
<tr>
<td>Patents Awarded</td>
<td>0</td>
</tr>
<tr>
<td>Patents Licensed</td>
<td>0</td>
</tr>
<tr>
<td>Software Licensed</td>
<td>0</td>
</tr>
<tr>
<td>Spin-off Companies Started (if applicable)</td>
<td>0</td>
</tr>
<tr>
<td>Degrees to NSEC Students</td>
<td></td>
</tr>
<tr>
<td>Bachelors Degrees Granted</td>
<td>0</td>
</tr>
<tr>
<td>Masters Degrees Granted</td>
<td>1</td>
</tr>
<tr>
<td>Doctoral Degrees Granted</td>
<td>1</td>
</tr>
<tr>
<td>NSEC Graduates Hired By</td>
<td></td>
</tr>
<tr>
<td>Industry</td>
<td></td>
</tr>
<tr>
<td>NSEC Participating Firms</td>
<td>0</td>
</tr>
<tr>
<td>Other US Firms</td>
<td>1</td>
</tr>
<tr>
<td>Government</td>
<td>0</td>
</tr>
<tr>
<td>Academic Institutions</td>
<td>0</td>
</tr>
<tr>
<td>Other</td>
<td>0</td>
</tr>
<tr>
<td>Unknown</td>
<td>0</td>
</tr>
<tr>
<td>NSEC Influence on Curriculum (if applicable)</td>
<td></td>
</tr>
<tr>
<td>New Courses Based on NSEC Research</td>
<td>1, 9**</td>
</tr>
<tr>
<td>Courses Modified to Include NSEC Research</td>
<td>10</td>
</tr>
<tr>
<td>New Textbooks Based on NSEC Research</td>
<td>0</td>
</tr>
<tr>
<td>Free-standing Course Modules or Instructional CDs</td>
<td>0</td>
</tr>
<tr>
<td>New Full Degree Programs (specify name of program and where implemented in footnote)</td>
<td>0, 2***</td>
</tr>
<tr>
<td>New Degree Minors or Minor Emphases (specify name of program and where implemented in footnote)</td>
<td>0</td>
</tr>
<tr>
<td>New Certificate (specify name of program and where implemented in footnote)</td>
<td>0</td>
</tr>
<tr>
<td>Information Dissemination/Educational Outreach</td>
<td></td>
</tr>
<tr>
<td>Workshops, Short Courses to Industry</td>
<td>0</td>
</tr>
<tr>
<td>Workshops, Short Courses to Others</td>
<td>1</td>
</tr>
<tr>
<td>Seminars, Colloquia, etc.</td>
<td>0</td>
</tr>
<tr>
<td>World Wide Web courses</td>
<td>0</td>
</tr>
</tbody>
</table>

* Printed, In Press, Submitted
** Implemented, Under Development
*** Implemented, Under Development. CBEN is contributing to two of the three new Sloan Professional Masters programs under development at Rice, the Nanoscale Physics program and the Environmental Decision Making program.
4. Mission and Broader Impact

Our mission is to create sustainable nanotechnology that improves human health and our environment. We do this by:

- **Fundamental examination of the ‘wet/dry’ interface** between nanomaterials and complex aqueous systems (Theme 1).
- **Interdisciplinary research** that combines nanochemistry, environmental and bioengineering to develop new nanotechnologies (Themes 2,3,4).
- **Innovative knowledge transfer activities** that recognize the central role that the academic entrepreneur plays in technology development.
- **Educational programs that develop teachers, students and citizens** who are well informed and enthusiastic about nanotechnology.

This mission is inspired by our conviction that nanomaterials have the potential to influence nearly all aspects of our society, much in the same way we now find polymers in nearly every technology we use. To realize this promise, organizations such as ours must develop the core curriculum, collaborative research and commercial technologies that lay the foundation for this revolution.

In our center’s relatively short five month existence we can claim many diverse research accomplishments ranging from a novel drug delivery scheme to new porous materials for water purification. **West** and **Halas** have developed nanoshell colloidal materials that absorb strongly in the near-infrared; these systems when incorporated into thermally sensitive polymers can be used to trigger the release of drugs. The idea is to use them as ‘intentional release’ drug packages to allow for patient controlled dosing of insulin, for example. **Wiesner** and **Colvin** have reported new types of membrane architectures for filtration based around template-assisted chemistries. By relying on the chemical tuning of colloidal crystallization and aggregation, templates of varying levels of porosity and pore size can be fabricated. With morphologies spanning multiple length scales (nanometers to micrometers), such architectures are well suited for filtration applications where surface fouling is a significant issue. Other research highlights include the visualization of a novel helical-ice form of water inside of nanotubes pores (**Ma, Smalley**), characterization of contaminant sorption onto model nanoparticles (**Tomson, Colvin**), and mechanically strong and transparent nanocomposites for injectable bone replacement (**Mikos, Barron**).

Our knowledge transfer activities have drawn large local audiences, and attracted national media attention. In December, CBEN was the co-host of a conference “The Environmental Implications of Nanotechnology: Perils and Values of This Emerging Technology”. This two day international event brought together environmental experts and nanotechnologists to discuss the intersection of these two disciplines. The Houston Chronicle, and the magazine Small Times, both covered the event. On March 1, CBEN will host a Rice Alliance Forum to allow center researchers to present their early stage technologies to interested investors and alumni. A graduate level course in entrepreneurial management for PhD scientists and engineers is also ongoing; in this venue, graduate students get introduced to business concepts and have the
chance to work with MBAs in developing business plans. These and other outreach activities are described in section 7 of this report.

Our educational initiatives have already begun to lay the groundwork for developing the nanotechnology workforce of the future. Highlights of these programs include the training of ninth grade science teachers both in content as well as pedagogy. This semester, the first portion of the program is well underway and fourteen teachers are participating in weekly nighttime courses co-taught by center participants and led by Dr. Ausman (Executive Director of Operations). Here, they learn basic concepts as related to the Texas ninth grade integrated physics and chemistry curriculum (IPC) in one hour, followed by a lecture from a NSEC researcher which relates to the current topic. Some of these teachers will participate in our longer training program, culminating in a semester sabbatical in the fall to improve pedagogical techniques and develop new curricular materials. In a pilot program this summer, this first portion of the teacher training described above will run as a three day workshop for teachers from Laredo, Texas, a predominantly hispanic school district. Another K-12 outreach program is our NanoKids™ program (Tour). This project teaches chemical principles at the middle school level; while this is a challenging prospect, the use of kid-friendly icons, NanoBoy and his friends, opens up the possibility of telling the story of chemistry through characters kids can relate to. At the undergraduate and graduate level new courses in nanotechnology are in the planning stages now. This nanocurriculum has taken on new directions with Rice’s Sloan Professional Master’s programs in nanotechnology and environmental decision-making. Together with these new degrees, and Rice’s Connexions program for web content development in science and engineering, these curricular efforts will have long-lasting impact. For more information on these highlights, and the larger educational outreach effort, please refer to section 6 in this report.
5. Research Accomplishments and Plans

5.1 Theme 1: Nanoscience at the Wet/Dry Interface

Theme Leader: Vicki Colvin
Personnel: 13 Faculty; 2 Undergraduate Students; 6 Graduate Students; 2 Postdocs; 1 Other Personnel

<table>
<thead>
<tr>
<th>Project</th>
<th>Leader</th>
<th>Investigators</th>
<th>Disciplines Involved</th>
<th>Number of Students and Post-docs</th>
<th>Current Year Budget</th>
<th>Proposed Budget</th>
</tr>
</thead>
<tbody>
<tr>
<td>Biological activity of bio-nanoconjugates</td>
<td>Vicki Colvin</td>
<td>Vicki Colvin and Cecilia Clementi (Chemistry), Kathlene Matthews and Kevin MacKenzie (Biochemistry and Cell Biology), Jennifer West (Bioengineering)</td>
<td>Inorganic chemistry Biochemistry Biology</td>
<td>1 Post-doc 2 Graduate Students 2 Undergraduates</td>
<td>$ 164,718</td>
<td>$ 207,759</td>
</tr>
<tr>
<td>Single-walled carbon nanotubes in complex aqueous media</td>
<td>Richard Smalley</td>
<td>Richard Smalley (Chemistry), Jianpeng Ma (Bioengineering), Boris Yakobson (Mechanical Engineering and Materials Science)</td>
<td>Chemistry Biology Physics</td>
<td>1 Post-doc 1 Graduate Student</td>
<td>$ 110,901</td>
<td>$ 114,228</td>
</tr>
<tr>
<td>Spectroscopic studies on carbon nanomaterials</td>
<td>Bruce Weisman</td>
<td>Bruce Weisman, Gustavo Scuseria, Richard Smalley (Chemistry)</td>
<td>Biology Chemistry Physics</td>
<td>1 Research Scientist 2 Graduate Students</td>
<td>$ 122,396</td>
<td>$ 126,068</td>
</tr>
<tr>
<td>Protein nanowires (seed)</td>
<td>Jason Hafner</td>
<td>Jason Hafner and Doug Natelson (Physics)</td>
<td>Physics Biology</td>
<td>1 Graduate Student</td>
<td>$ 51,600</td>
<td>$ 40,103</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$ 449,615</td>
<td>$ 488,158</td>
</tr>
</tbody>
</table>

The aim of this theme is to develop the basic science needed for the rational design and exploitation of the wet/dry interface. By wet/dry interface we mean the interface between an inorganic nanomaterial, the ‘dry’ side, and a biological system, the ‘wet’ side. Controlling this interface is essential for bringing nanotechnology into bioengineering (theme #2) and for ensuring nanotechnology has a positive environmental impact (theme #3).

The wet/dry interface is a challenging problem for scientists. Nanomaterials are, in most cases, foreign materials in biology. How they affect biochemical and cellular processes is a crucial question, yet difficult to predict from standard biological or chemical considerations. The first project in this theme aims to develop a more general understanding of these issues. Bio-nano hybrid materials are evaluated for their biological activity and cellular interactions, and the results correlated with the physical properties of the nanostructures. Projects 2 and 3 focus on the formation of biologically active carbon single walled nanotubes (SWNT). Because such materials are very hydrophobic, their solubilization in water is a core issue (Project 2) as is their detection in aqueous solvents (Project 3). Biology also provides natural nanostructures that when connected to the outside world through a ‘dry’ contact hold great potential for nanotechnology. A seed project exploits the protein actin as a nanowire capable of biological recognition and ultimately sensing (Project 4). Taken together, these programs will harness biological processes for nanotechnology with the aim of developing a “wet nanoscience” that provides the scientific core for environmental and biological nanotechnologies.

5.1.1 Biological activity of bio-nanoconjugates

Investigators: Colvin, Matthews, MacKenzie, Clementi, West
The objective of this project is to develop a fundamental understanding of the biological activity of bionanoconjugates. This issue is evaluated at both a biochemical level, where the recognition processes of Lac-Repressor protein- nanocrystals complexes for DNA are measured, as well as at a cellular level where nanoparticle uptake into both mammalian and bacterial cells is correlated with bionanoconjugate size and shape. These efforts were motivated in large part by the needs of bioengineers using bionanoconjugates (Theme #2) and by the importance of bio-nano interactions in determining environmental impact (Theme #3). The ability to turn on and off the uptake of a bionanoconjugate into a cell, for example, allows for sophisticated drug delivery schemes. However, little is known about the process by which cells take up nanoparticles with sizes below 100 nm. Likewise, bionanoconjugates often have a reduced activity relative to native biomolecules, yet little can be done to solve this problem since no general understanding of the activity of bionanoconjugates exists. This research seeks to identify what factors, such as nanoparticle size or shape, contribute to the reduced activity of biomolecules.

Over the last few months, this team has focused on the first task for both the biochemical and cell studies of bionanoconjugates: the production of well controlled nanocrystal-biomolecule conjugates (Colvin). For this program it is essential that we control nanocrystal size and shape quite precisely, and that we have a separation scheme for forming populations of nanocrystals that have similar surface chemistries. We chose gold nanocrystals as our model system since there exist a handful of reports of synthetic strategies for forming these nanoparticles bound to biomolecules. Our current strategy relies on the borohydride reduction of gold-surfactant complexes; this reaction produces relatively monodisperse (σ ~ 15%) spherical and rod-like particles depending on the reaction conditions. We are exploring several capping agents which present ammonium and phosphate functionalities in order to produce nanocrystals that remain unaggregated in the high ionic strength buffers needed for the biochemical assays, as well as for cellular growth. We have also developed the means to couple proteins directly to particle surfaces using protein cross-linking compounds which have free thiols; these complexes allow specific amino acids to be anchored to particle surfaces. Gold nanocrystals will be tethered to ssDNA using established methods, and will form duplex DNA by adding the complementary strand. Single strands with known operator sequences will be purchased commercially and radiolabelled with γ-[32P]ATP and polynucleotide kinase. Finally, for our studies it is important to separate nanocrystals which may be bound to multiple biomolecules, or nanocrystals which become bound to each other, from those that are single bionanoconjugates. High pressure liquid chromatography (HPLC) using size exclusion columns is effective at separating gold nanocrystals based on the length of the capping group’s alkyl chains. We are adapting this method for water soluble bio-nanocrystals to allow for pure populations of bionanoconjugates to be produced.

After this preparative chromatography biomolecule coverage and flexibility will be assessed (MacKenzie) with 1D and 2D NMR experiments. The effect of these gold nanocrystals on biochemical recognition will be the subject of investigations over the next year (Matthews). This group has expertise with measuring the relative binding affinity and kinetics of the recognition process between LacR and DNA. The standard methods will be adapted for these particles, and/or surface plasmon resonance will be used to detect binding. These experimental studies will be complemented by computational models of the recognition process (Clementi). Studies of
cellular uptake of particles will also be started in the next year, once well characterized and separated bionanoconjugates are available (West).

5.1.2 Single-walled carbon nanotubes in complex aqueous media
Investigators: Smalley, Ma, Yakobson

This project’s goals are to understand and tailor the interactions of single-walled carbon nanotubes (SWNTs) with water itself and with complex aqueous systems such as polymer- or surfactant-based solubilizers and biomolecules. Smalley is further developing techniques to render individual SWNTs water soluble through supramolecular association with surfactants and alternately with water-soluble polymers, and is targeting high solubility under typical biological conditions.

Collaborative efforts with Professor Angela Belcher of UT Austin have focused on use of phage display libraries to discover specific protein sequences that have strong binding affinity to SWNTs. Early results have discovered several of these specific sequences that are quite effective. Extensive further work is planned using individual nanotubes prepared in solution.

Molecular dynamics simulations were performed on nanotubes segments of various diameters submerged in water (Ma). The results show water molecules can exist inside the nanotube segments, and the water molecules inside the tubes tend to organize themselves into a perfectly hydrogen-bonded network, i.e., solid-like wrapped-around ice sheets. The disorder-to-order transition of these ice sheets can be achieved purely by tuning the size of the tubes. The results suggest the nanotubes have the potential to be used as proton-conducting pores for a variety of biological applications. Future plans include studying the interactions of water with other portions of the nanotubes as a function of size, helicity, and end-cap derivitization. Once that is well-understood, polymer-wrapped SWNTs of the types produced by Smalley will be investigated.

Figure 5.1.1 Helically-ordered water phase observed in molecular dynamics simulations under ambient conditions in the center of carbon nanotubes.
Simulations have also been performed on a fullerene-specific antibody (Ma), providing a detailed description of the active-site’s interactions with the molecule (Figure 5.1.2). This proof-of-concept simulation is but the first step in a series of simulations targeting interactions between biomolecules, such as those developed in the Belcher collaboration, and larger fullerenes such as SWNTs.

The structural and dynamic properties of systems containing nanotubes and lipid molecules are under investigation by similar methods (Ma). We are considering two situations: one with segments of nanotubes embedded in phospholipid bilayers and another with the nanotubes coated in SDS (sodium dodecylsulfate) micelles.

Yakobson is in the process of calculating the effects of solvent-immersion on the vibrational modes of SWNTs, providing vital information for interpreting the Raman spectra of nanotubes in these media.

5.1.3 Spectroscopic studies on carbon nanomaterials
Investigators: Weisman, Scuseria, Smalley

Two primary hurdles in manipulating carbon nanotubes are generating individually-dispersed suspensions/solutions, and experimentally observing that the resulting dispersions are in fact individually-dispersed. These two goals represent gateway technologies to liquid-phase separations of the tubes, high-yield chemical derivitizations, and eventually assembly into larger structures. Traditional methods for measuring SWNT dispersion quality rely on probe microscopy techniques, thus suffering from slow throughput and a disconnect between the sample of interest and that being directly probed.

A recent breakthrough by Weisman and Smalley reveals that SWNTs dispersed in a surfactant/water mixture are strongly fluorescent, but only if the tubes are individuals rather than bundles or ropes. This provides a rapid, effective assay for dispersion quality. The details of this newly-observed phenomenon are currently under investigation, but early results suggest that the observed fluorescence spectra do not agree with theoretical predictions. Their electronic absorption spectra, near-infrared photoluminescence spectra, and resonance Raman spectra will be measured in an attempt to develop sensitive, species-specific methods for detecting and characterizing carbon nanotubes in a variety of environments. Scuseria will calculate the electronic structures of a series of nanotubes (different diameters, helicities, etc.) in an effort to explain the observed results. The computational methods to be employed include hybrid density
functional theory with periodic boundary conditions and large Gaussian basis sets. These calculations will provide accurate estimates of the nanotubes band gaps that can be used in rationalizing the fluorescence data and provide means to identify specific tubes. Scuseria will also carry out tight-binding density functional theory calculations of the breathing modes of single-wall carbon nanotubes of different diameters and helicities. Previous calculations on fullerenes like C$_{60}$ have shown that these methods are capable of reproducing Raman active vibrational modes within a few wavenumbers. Thus, it is expected that the results of these calculations may be used as fingerprints for identifying different classes of individual tubes. These studies may be extended to include calculations of Raman frequency shifts of solubilizing polymers relative to those of the free polymer.

5.1.4 Protein Nanowires

Investigators: Hafner, Natelson

The objective of this work is to study electrical transport through protein nanowires in aqueous environments, and to assess whether sensors based on conductivity changes could be developed. This project is inspired by a 1994 literature report of ionic conduction along actin filaments (F-actin) due to the dense cloud of counterions on their surface. This work was limited in its scope because of the to the large length scale (60 micron) of the actin and the poorly defined electrical interface (patch clamp pipettes). With new nanometer-scale tools such as E-beam lithography and atomic force microscopy (AFM), we will study ionic transport in F-actin over a smaller length scale and try to understand the phenomenon in terms of fluctuating counterion concentrations. We will engineer a localized interface for the transmission of current from electron transport in the nano-electrodes to ionic transport in the protein nanowire. Finally, we will study the effect of bound analytes on the ionic transport.

The observation that filamentous proteins such as F-actin allow electrical transport along their length is interesting both for biology as well as nanotechnology. F-actin and other protein filaments make up the cytoskeleton, which gives the cell structural support, controls cell shape and movement, and organizes sub-cellular components. It is possible that the cytoskeleton also plays a role in intracellular signaling, and these ionic currents may represent a medium for these signals. On practical note, protein wires such as F-actin could be employed as all-electrical biosensors by measuring changes in their dynamic conductance upon specific binding of analytes that would perturb the counterion concentration around the wire. Planar field effect transistors (FETs) operate on a similar principal, but suffer from limited sensitivity since the analyte must cover the two-dimensional gate structure. Recently, silicon nanowire based biosensors were introduced which are highly sensitive due to their one-dimensional nature and small size. F-actin biosensors would enjoy the same benefits, but avoid the costly production and environmental impact of semiconductor nanowires.

Purified actin is commercially available and the conditions under which it polymerizes into F-actin have been extensively studied. F-actin solutions will be prepared and the concentration and time
parameters for their deposition onto silicon wafers will be studied in solution by AFM (Hafner). Gold nanoelectrode patterns on silicon wafers will be prepared by E-beam lithography (Natelson). Nanoelectrodes with separations ranging from several microns to fewer than 50 nm will be studied to evaluate how the filament length affects transport. These patterns will then be imaged by AFM under an aqueous solution of F-actin. Continuous AFM imaging and interelectrode conductance monitoring will reveal when an actin filament has bridged the electrodes. At this point, dc ionic transport measurements will proceed by applying voltage pulses to one electrode and measuring the resulting current at the other electrode with a patch clamp amplifier. In addition to pulses, the AC current response of the actin filament will be studied using lock-in amplifier techniques. This combination of nano-electronics and fluid AFM imaging of proteins will require the combined expertise of Hafner and Natelson's research groups, and represents an interesting example of research at the wet-dry interface.
5.2 Theme 2: Nanomaterials in Bioengineering
Theme Leader: Jennifer West
Personnel: 6 Faculty; 4 Undergraduate Students; 4 Graduate Students; 1 Postdocs

<table>
<thead>
<tr>
<th>Project</th>
<th>Leader</th>
<th>Investigators</th>
<th>Disciplines Involved</th>
<th>Number of Students and Post-docs</th>
<th>Current Year Budget</th>
<th>Proposed Budget</th>
</tr>
</thead>
<tbody>
<tr>
<td>Metal nanoshells in bioengineering</td>
<td>Jennifer West</td>
<td>Jennifer West and Rebekah Drezek (Bioengineering), Naomi Halas (Electrical and Computer Engineering)</td>
<td>Physics, Chemistry, Bioengineering</td>
<td>1 Post-doc, 2 Graduate Students, 2 Undergraduates</td>
<td>$226,353</td>
<td>$250,226</td>
</tr>
<tr>
<td>Nanocomposites for bone replacement</td>
<td>Antonios Mikos</td>
<td>Antonios Mikos (Bioengineering), Andrew Barron and Jeffrey Hartgerink (Chemistry)</td>
<td>Chemistry, Bioengineering, Materials Science</td>
<td>2 Graduate Students, 2 Undergraduates</td>
<td>$99,259</td>
<td>$142,340</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td></td>
<td>$325,612</td>
<td>$392,566</td>
<td></td>
</tr>
</tbody>
</table>

There may be no division of engineering that places greater constraints on material characteristics than bioengineering. Not only do biomaterials have to meet the stringent performance requirements demanded of specific applications, but they must also be biocompatible and often biodegradable. The research in this theme aims to exploit the unique properties of nanomaterials to provide solutions for challenging bioengineering problems. The first project area leverages the extremely small size and optical tunability of isolated nanoparticles. Such features are of great value in applications ranging from drug delivery to optical imaging. The second project area uses nanochemistry to influence the properties of solid materials designed for tissue replacement. As illustrated in the discussion below, even at relatively low levels of incorporation, nanoparticles can significantly enhance the properties of bone replacement.

5.2.1 Metal nanoshells in bioengineering
Investigators: West, Halas, Drezek

**Drug Delivery.** Modulated drug delivery implants, systems that allow sustained release of a drug with controlled and changing dosage profiles, have long been the “holy grail” of drug delivery research. Temperature-sensitive polymers, such as poly(NIPAAm-co-AAm), have been investigated for use as modulated drug delivery systems, but a safe, convenient, and effective means of controlling the temperature of such implants has been lacking. However, since tissue is essentially transparent to near infrared light (in the range of 800-1300 nm), nanoshell-polymer composites, with nanoshells designed to strongly absorb near infrared light combined with a thermally responsive polymer, may represent an implantable system where drug release rates can be externally modulated by exposure to light. Demonstrating this phenomenon, irradiation of insulin-loaded nanoshell/hydrogel composites with a diode laser (821 nm) dramatically increases the rate of drug delivery. Pulsatile drug delivery profiles were achieved by periodic irradiation. Additionally, using a glucose uptake assay with L929 cells, we have demonstrated that insulin released from this system maintains its bioactivity.
Composites of thermally sensitive hydrogels and optically active nanoparticles have been developed for biomedical applications including photothermally modulated drug delivery and optically controlled microfluidics systems. Copolymers of N-isopropylacrylamide (NIPAAm) and acrylamide (AAm) exhibit a lower critical solution temperature (LCST) slightly above body temperature. When the copolymer temperature exceeds the LCST, the hydrogel collapses, due to a transition of the polymer chains from a coil to globule state. Gold nanoshells that strongly absorb light at ~820 nm have been incorporated into poly(NIPAAm-co-AAm) hydrogels for the purpose of initiating a temperature change in response to light; light at this wavelength is transmitted through tissue with relatively little attenuation, is absorbed by the nanoshells and converted to heat. These nanoshell-hydrogel composites collapse dramatically in response to irradiation with a near infrared diode laser (821 nm). This collapse response is completely reversible, allowing repetitive manipulation of the composite materials as shown in Figure 5.2.1.

In addition to uses in drug delivery, these optically responsive composites have a number of other potential applications. One of particular interest is to use these materials as optically controlled valves in microfluidics devices for cell sorting and bioassays. We have fabricated composites that respond separately to different wavelengths of light (532 nm and 821 nm). The materials that respond to green light are composites of poly(NIPAAm-co-AAm) and gold colloid, while the near infrared-responsive materials are nanoshell composites as described above. The extinction spectra of the two composite materials are shown in Figure 5.2.2. These materials can be separately controlled, depending upon the wavelength of light used to illuminate the

---

**Figure 5.2.1** Nanoshell composites were exposed to four 10 minute irradiation cycles as the degree of swelling was monitored. The responses of this system were reversible and repeatable.

**Figure 5.2.2** Optical extinction profiles for composites formed using gold colloid (black line) and gold nanoshells (grey line).

**Figure 5.2.3** (Left) Responses to 821 nm irradiation. Only the nanoshells composite undergoes collapse. (Right) Responses to 532 nm irradiation. Only the colloid composites collapse.
system, as shown in Figure 5.2.3. We have recently formed these composites as posts within microfluidic channels and have demonstrated collapse of the posts, thus allowing flow through the channel, only in response to the appropriate wavelength of light. Using additional nanoshells and other nanomaterials, it should be possible to develop multiple components that can be independently activated to control flow patterns through microfluidics devices.

**Optical Imaging with Nanoshells.** There is a significant clinical need for novel methods for detection of precancerous conditions which offer improved sensitivity, specificity, and cost-effectiveness. In recent years, a number of groups have demonstrated that optical spectroscopic and imaging approaches are valuable in addressing this need. However, in many cases, these optical technologies are limited by the inherently weak optical signals of endogenous chromophores and the subtle spectral differences of normal and diseased tissue. The project described leverages recent advances in nanoparticle technologies to develop innovative contrast agents which can be optically interrogated using noninvasive approaches and targeted to specific molecular signatures of disease. The contrast agents proposed - nanoshells and nanoemitters - possess ideal optical and chemical properties for optical imaging. The optical response of these particles can be precisely and systematically varied over a broad band including the visible and infrared spectral regions. Moreover, the nanoparticles are highly biocompatible and proteins (such as antibodies) are readily conjugated to their surfaces. In this interdisciplinary project, we bring together expertise in nanotechnology and biophotonics to develop nanoparticle-enhanced optical imaging technologies which may provide a significant breakthrough in the detection of precancerous conditions.

In Year 1 of this project we have focused on development of the software design tools required to design optimized optical contrast agents (Drezek). As a simple demonstration of the type of information the proposed modeling approach can provide, we used our preliminary models to simulate changes in diffuse reflectance of epithelial tissue at 600 nm after topical application of optical contrast agents. First, an inverse analytical approach was used to engineer nanoparticles optimized for scattering and absorption properties. A scattering particle with a core radius of 35 nm and shell thickness of 37 nm, and an absorbing particle with a core radius of 35 nm and shell thickness of 16 nm yielded optimal results (scattering and absorption efficiency of 2.84 and 3.606, respectively). We then used a Monte Carlo to calculate diffuse reflectance as a function of the concentration of the particles with the tissue using published optical properties of

![Figure 5.2.4 Predicted changes in diffuse reflectance remitted from epithelial tissue as a function of concentration of scattering nanoparticles (left) and absorbing nanoparticles (right).](image-url)
epithelial tissue at 600 nm. As shown in Figure 5.2.4, the increase in reflectance generated by scattering nanoparticles and the decrease in reflectance generated by absorbing nanoparticles, are changes large enough to be easily measured using standard instrumentation (a SNR of 100 is reasonably achieved). In preliminary experimental studies we have demonstrated binding of several hundred nanoparticles per cell. The concentrations used in the simulations were based on this information. The data shown are based on a preliminary model with a number of limiting assumptions. We do not intend the data to be treated as exact quantifications of contrast but rather to demonstrate that it is reasonable to expect detectable changes will result from the nanoparticle-based contrast agents.

Physically constructing a wide range of proposed nanoparticle configurations and testing each configuration in both non-biological and biological phantoms requires an intensive commitment of time and resources. We seek to reduce the required number of iterations by developing computational tools which can quickly compare the predicted effectiveness of a large number of nanoparticles in order that we may concentrate our laboratory efforts on those most likely to provide optimum results. Specifically, we will engineer optimally scattering and absorbing particles at wavelengths within the visible and IR spectral regions chosen to minimize interference from biological chromophores and based on the availability of convenient light sources. More generally, we believe that biological applications of nanoparticle technologies will expand dramatically in the next decade and the design tools developed for this project will be directly relevant to many other nanotechnology problems.

To fully develop the potential of nanoparticles as contrast agents for optical imaging, we will use this novel class of exogenous contrast agents to address the clinically important problem of detection of pre-invasive neoplasias. Our specific activities will include the design of nanoparticle-based optical contrast agents; the development of software simulations tools for nanoparticle-based optical imaging; and the evaluation of nanoshell and nanoemitter contrast agents in biological models. These activities will test the hypothesis that nanoparticles can be engineered to function as visible and near IR contrast agents for optical imaging. Furthermore, the tools and contrast agents developed in this project will be broadly applicable to other emerging diagnostic and therapeutic biophotonics applications. Finally, we will use the interactive light propagation software in undergraduate and graduate courses in biomedical optics and broadly disseminate it to the optics community for educational purposes.

5.2.2 Nanocomposites for bone replacement

Investigators: Mikos, Barron, Hartgerink

Composites that incorporate chemically functionalized nanoparticles realize significant improvements in physical properties such as toughness, impermeability, and chemical resistance and flexibility. In this project, materials chemists with expertise in the production of polymeric matrices with nanoscopic features team with a bioengineer specializing in bone replacement scaffolds. Over the past few months, commercial nanoparticles have been used to confirm the hypothesis that nanoparticles can enhance the properties of bone replacement polymers (Mikos). In the next year, smaller particles tailored at their surfaces to anchor to the polymer backbone (Barron) will be tested in a similar fashion. Also, the expertise of a new chemistry professor,
Hartgerink, will provide for even more sophisticated design of the nanoscopic architecture of polymer replacement materials.

The near-term objective of this work was the investigation of the mechanical properties of poly(propylene fumarate)/poly(propylene fumarate)-diacrylate (PPF/PPF-DA) networks which incorporated nanoalumina (Al₂O₃) particles. These polymers alone have been demonstrated to be effective, biocompatible scaffolds for bone replacements. We have found that nanocomposites of alumina and poly(L-lactic) acid (PLA) have demonstrated more than a three fold increase in the bending modulus of the pure polymer. In addition, these composites showed improved osteoblast attachment while reducing fibroblast adhesion. The incorporation of these alumina nanoparticles has provided desirable mechanical and bioactive properties for bone tissue engineering applications.

PPF, a viscous liquid, can be crosslinked with poly(propylene fumarate)-diacrylate (PPF-DA) to form a solid, biodegradable material. The crosslinking reaction can be carried in situ allowing for the polymer to be injected into a bone defect and then conform to the defect shape. A nanocomposite of alumina and PPF/PPF-DA would be ideal for an injectable substrate for bone tissue engineering. We hypothesized that incorporation of the nanophase into these PPF/PPF-DA networks will demonstrate similar improvements to the mechanical properties and bioactivity as accomplished with PLA.

Nanocomposites were formed by photo-crosslinking a mixture of alumina particles in the polymer phase. Briefly, measured quantities of alumina (0, 10, 30, and 50 wt%) were added to PPF/PPF-DA and the slurry was thoroughly stirred. The photo-initiator (bis-(2,4,6 trimethylbenzoyl) phenylphosphine oxide (BAPO)) was administered to the mixture in a 0.1 g/ml solution of CH₂Cl₂ so that the initiator content was 0.3 wt%. The paste was then placed under vacuum (< 1 mmHg) for 5 minutes in order to remove any bubbles. The mixture was then poured into teflon molds and exposed to UV light for 30 minutes in order to crosslink the nanocomposite. Test specimens of a bar shape with dimensions 2 mm x 6 mm x 35 mm were prepared for 3-point bend testing.

Bend testing was carried out on an 858 Bionix MTS test machine equipped with a 3-point bend fixture. The specimens were tested at a span length of 25 mm and were subjected to a load at the midpoint moving at a crosshead speed of 1 mm/min until fracture. The load and displacement were recorded throughout and utilized to obtain the bending stress vs. strain curve. The bending modulus was calculated as the slope of the initial linear portion of the curve and the bending strength was determined as the maximum stress.

For the alumina concentrations examined in this study, the bending modulus and strength ranged from 1367 ± 144 to 1906 ± 317 MPa and 29 ± 5 to 38 ± 7 MPa, respectively (Figure 5.2.6). There was an increase in bending modulus for nanocomposites of 10 and 30 wt% alumina compared to pure PPF/PPF-DA networks (p < 0.05). The fall-off in the properties with increased concentrations of nanoparticles is due to the poor characteristics of commercial nanoalumina. These particles are large enough (d > 50 nm) that at high concentrations they scatter light in our plugs and interfere with photopolymerization. In addition, their surface preparation is not tailored to anchor them to the polymer so at large concentrations they may aggregate which can
result in a lower modulus as observed in the 50 wt% composites. There was no effect of alumina content on the bending strength.

We are currently examining the compressive mechanical properties of the alumina/PPF/PPF-DA nanocomposites. Our initial attempts to form cylindrical specimens of 6 mm diameter were complicated by incomplete crosslinking of the polymer. The resulting samples were hollow cylinders of approximately 1 mm thickness with the uncrosslinked ceramic/polymer slurry inside. Apparently the alumina nanoparticles prohibit the penetration of UV light into the interior of the specimen. Interestingly, when forming porous scaffolds of the same 6 mm diameter by the porogen leaching technique, the polymer phase is crosslinked throughout. Mechanical evaluation of the effect of alumina concentration on the compressive properties of porous nanocomposite scaffolds is currently underway.

With smaller alumina nanoparticles from Barron, scattering losses should be minimized to enable the production of superior nanocomposites. These alumina nanoparticles are termed carboxylate-alumoxanes. The choice of carboxylic acid allows for chemically functional groups, such as OH and NH, to be available for surface chemistry. We have demonstrated that lysine-alumoxane reacts with a range of acyl chlorides. This is the first step towards incorporation into poly(propylene fumarate) (PPF) polymers. We propose to investigate the formation of PPF-alumoxane composites and determine the effect of the alumoxane on the tensile and torsional strength of the composite. In addition, we will ascertain the effect of the alumoxane on the porosity of the polymer composite.

The alumina nanoparticles are expected to enhance the strength of bone replacement materials; however, equally important issues are the development of micro- and mesoporosity in the polymer scaffolds to allow for nutrient transport as well as the tailoring of polymer surface chemistry for biological recognition. Over the next year, the expertise of a newly hired professor in chemistry, Dr. Hartgerink, will be brought to bear on these problems. He will focus on the synthesis of nanostructured materials for tissue engineering and regeneration. These materials are designed to enhance the healing and growth of tissues in part by mimicking the structure and chemistry of

![Figure 5.2.5 The effects of alumina concentration on the bending modulus and strength of PPF/PPF-DA nanocomposites.](image-url)
the natural environment that cells grow in - the extracellular matrix. The structures that are found in the extracellular matrix are too large (many nanometers in dimension) to synthesize by traditional chemical means. Hartgerink will develop the principles of supramolecular chemistry to self-assemble these large structures from smaller, easier to prepare parts. The structural and chemical control afforded by such a strategy will impart an important biological activity to these implant materials. Such features could be used to cause preferential growth of particular cell lines, to promote differentiation of stem cells, or to deliver drugs such as antibiotics and immune suppressants.
5.3 Theme 3: The Environmental Implications of Nanotechnology

Theme Leader: Mark Wiesner
Personnel: 8 Faculty; 1 Undergraduate Students; 7 Graduate Students; 2 Postdocs

<table>
<thead>
<tr>
<th>Project</th>
<th>Leader</th>
<th>Investigators</th>
<th>Disciplines Involved</th>
<th>Number of Students and Post-docs</th>
<th>Current Year Budget</th>
<th>Proposed Budget</th>
</tr>
</thead>
<tbody>
<tr>
<td>Core Projects</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nanostructured membranes and their applications</td>
<td>Mark Wiesner</td>
<td>Mark Wiesner (Environmental Science and Engineering), Andrew Barron and Vicki Colvin (Chemistry)</td>
<td>Physical Chemistry, Fluid Mechanics, Risk Assessment, Separations Science</td>
<td>1 Post-doc 3 Graduate Students 1 Undergraduate</td>
<td>$ 270,543</td>
<td>$ 278,659</td>
</tr>
<tr>
<td>Polymer flow on the nanoscale</td>
<td>Matteo Pasquali</td>
<td>Matteo Pasquali (Chemical Engineering), Anatoly Kolomeisky (Chemistry)</td>
<td>Fluid Mechanics, Physical Chemistry, Rheology</td>
<td>1 Graduate Student</td>
<td>$ 45,677</td>
<td>$ 85,147</td>
</tr>
<tr>
<td>Nanomaterial fate and transport in the environment</td>
<td>Mason Tomson</td>
<td>Mason Tomson, Mark Wiesner, and Joseph Hughes (Environmental Science and Engineering), Vicki Colvin and Richard Smalley (Chemistry)</td>
<td>Physical Chemistry</td>
<td>1 Post-doc 3 Graduate Students</td>
<td>$ 208,191</td>
<td>$ 214,436</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$ 524,411</td>
<td>$ 578,242</td>
</tr>
</tbody>
</table>

The research in this section endeavors to guarantee that nanotechnology emerges as a positive, powerful tool for improving our environment. Two project areas look at the fabrication and applications of membranes in which nanochemistry has provided fine control over pore density, morphology and surface chemistry (5.3.1, 5.3.2). Chemistry, modeling and environmental technology are blended in these collaborative programs aimed at the production of better water treatment systems, catalytic supports and filters. The third project area measures the potential for nanostructures to influence the fate and transport of organic and inorganic contaminants in water (5.3.3). The physical and chemical adsorption of contaminants to nanoparticle surfaces are quantified in this work, and related to basic properties of the nanoscale solid. This information makes it possible to anticipate the unintended consequences of passive sorption onto nanoparticles in waste streams; in addition, it also provides a springboard for the intentional design of separable nanoparticles able to sequester waste products. Future work in this area will expand to include the interaction of nanoparticles with biological systems, such as bacteria, so as to enable the center to develop a comprehensive environmental impact statement for nanomaterials.

5.3.1 Nanostructured membranes and their applications
Investigators: Wiesner, Barron, Colvin

Porous materials, or membranes, find wide use in environmental technology as water filters, catalytic supports and sensors. In this project, the expertise of materials chemists (Colvin, Barron) specializing in nanochemistry is leveraged in the development of new membranes for environmental technology (Wiesner). During the first several months of this project, efforts have focused on three areas: 1) Computational simulations of template formation from nanoparticle deposition, 2) Experimental exploration of the variability in template morphology as a function of nanoparticle surface chemistry, and 3) Formation of ferroxane nanoparticle films deposited on macroporous supports.
Detailed control over the porosity and architecture of a membrane is essential in defining its function. Computational work which uses a Monte Carlo code to simulate the growth of a deposit has suggested strategies for creating nanoparticle templates with a wide range of morphologies through tuning of the interparticle potentials (Wiesner). Under conditions of low particle-particle interaction, templates are created of relatively high density and great regularity in packing. As particle-particle interactions become more favorable, templates become more porous. (Figures 5.3.1, 5.3.2)

Experimental work has shown that these theoretical expectations are realized and can be used to create deposits with a wide range of morphologies. By using these systems as templates for producing inverted porosity, we will create interesting porous architectures with large porosity and good mechanical strength (Colvin). These membranes will be the starting point for evaluating catalysis, water filtration and surface enhanced raman scattering from complex, porous surfaces.

Related work has proceeded in the area of nanoparticle precursors for active membrane supports. Following from our previous work on alumoxane membranes (Barron, Wiesner), we are now
using ferroxane nanoparticles a precursors for membranes with metallic and catalytic character (Figure 5.3.3). They are first deposited on a porous substrate and sintered to form an iron-based ceramic membrane. Results to date appear very promising in that the sintered layers retain good structural integrity after thermal treatments. To lower the resistance of this membrane, we are working to reduce the thickness of the initial deposit.

Our specific goals for the next year include first the development of templated membranes from nanoparticle deposits (Colvin, Wiesner). Various strategies for introducing/polymerizing monomer to form membranes will be investigated as will variations of polymer formulation to form templated membranes with tailored surface chemistries. Membranes will be characterized in terms of selectivity, permeability and susceptibility to fouling. The next is the refinement and testing of ferroxane-derived ceramic membranes in filtration and catalysis. We are particularly interested in the basic characteristics of these new systems and will characterize their molecular weight cutoff, permeability, pH tolerance, and reactivity for conversion of species via Fenton’s pathways (Wiesner, Barron). Finally, the surfaces of the low density deposits are ideal for sensing applications. The surface-enhanced raman effect will be evaluated for such templated structures treated with silver nanoparticles. If this approach appears promising, we will investigate whether these materials can be developed as sensors for selected environmental contaminants (Barron, Wiesner, Colvin).

5.3.2 Fluid flow on the nanoscale
Investigators: Pasquali, Kolomeisky

Computational modeling is an essential component both for the design of better membranes, and for the development of separation tools for nanomaterials. In this work we are developing a model of flow of individual polymer molecules through nanopores. This simple system is of great relevance to membrane design, both in developing better separations for nanomaterials as well as in the prevention of fouling, in which large naturally occurring macromolecules block the pores of membranes.

In the past few months, a statistical mechanical theory of polymer translocation through long nanopores has been developed (Kolomeisky). The explicit results for translocation times of polymers are calculated for general sets of parameters. It is shown that the translocation dynamics for long polymers (larger than the nanopore size) is different from that of relatively short polymers (smaller than the nanopore size). In addition, the voltage dependence of polymer transport is described by using simple phenomenological approach. Our results are in good agreement with available experimental data on voltage-driven DNA translocation through a-hemolysin channel.

Concurrently, the transient and steady behavior of dilute solutions of worm-like polymer in shear flow have been studied by Brownian Dynamics (Pasquali). The effects of the ratio of contour and persistence length and of shear rate on the conformational and material properties have been analyzed. We find that semiflexible molecules differ qualitatively from flexible ones; in flow, they shrink rather than expanding, and assume highly bent configurations. We propose new scaling laws for zero shear viscosity and zero first normal stress difference that account for the effect of molecular stiffness. We also present a mastercurve for material functions of
semiflexible chains, and we identify two different power law regimes depending on the relative value of hydrodynamic and bending forces.

We are currently investigating the effects of nanopore geometry and polymer flexibility on translocation dynamics. We are using a unique combination of high-performance computing and stochastic simulations (the expertise of Pasquali), and equilibrium as well as non-equilibrium statistical mechanics (the expertise of Kolomeisky). In this way a computational engineer focused on the macroscopic features of matter (Pasquali) and a theoretical chemist versed in the microscopic world (Kolomeisky) meet on the nanometer scale. We will investigate the effect of interactions between nanopore walls and polymer on overall transport across the pore. Finally, we will investigate the translocation of polymers into spherical objects. We plan to include all relevant physical effects in our stochastic models, such as external fields (e.g., electrophoretic potentials), polymer excluded volume, hydrodynamic interactions, and polymer chain stiffness. If warranted, we will investigate the novel regime where the polymer dynamics and the fluid flow in the micropore are tightly coupled and the standard decoupling techniques do not apply.

5.3.3 Nanomaterial fate and transport in the environment
Investigators: Tomson, Wiesner, Hughes, Colvin, Smalley

The production of significant quantities of anthropogenically-derived nanomaterials will inevitably result in the introduction of these materials to the atmosphere, hydrosphere, and biosphere. The fate, persistence, paths of exposure, and interaction with other chemical species are key issues to be addressed in this research. We study two classes of anthropogenically-derived nanomaterials, TiO_2 nanocrystals and carbon nanotubes, and compare the properties of these materials with those of nanoparticles currently present in a surface water and groundwater environment. Our focus to date has been on two key problems: 1) adsorptive interactions of inorganic and organic pollutants with TiO_2 and carbon nanotubes; and 2) effects of nanoparticles on nucleation of common inorganic constituents of natural water. Over the next year we will begin to consider two additional issues: the mobility, aggregation of nanoparticles and their interaction with biological systems such as bacteria.

Initial research has been devoted to understanding the adsorption potential of common environmental pollutants (both organic and inorganics) to nanomaterials (sub-micron sized buckminsterfullerene and anatase) (Tomson). In particular the sorption of naphthalene and cadmium to the above two nanomaterials were studied. Both of these pollutants are on EPA's priority pollutant list, therefore, they have been studied extensively by the PI and others on their sorption to natural sediments. In Figure 1a is plotted the sorption isotherm of naphthalene to buckminsterfullerene (C_{60}). The majority of the research has been focused on methods development and will be used with nanoparticles provided by Colvin during the next period. The sorption isotherm can be fitted with a Freundlich isotherm (q (mg/Kg C_{60})= 10^{3.34} \cdot C^{0.48} (mg/L)). Also plotted in Figure 1a is the sorption isotherm of naphthalene to a typical soil as predicted from the K_{oc}/K_{ow} relationship. The sorption of naphthalene to buckminsterfullerene is similar to the sorption to soil on a per carbon base, except that the sorption isotherm is highly nonlinear. In Figure 1b is plotted the sorption isotherm of cadmium to anatase and a natural sediment from Utica, NY (pH 6.2). The sorption data are fitted with Langmuir isotherms. Interestingly, sorption of Cd to anatase is significantly stronger than that of Utica soil on a per weight base, with a
Langmuir sorption maximum approximately 5 time larger for anatase than for Utica sediment. The surface area of Utica sediment is 3.9 m²/g. The surface area, maximum charge density, pzc of anatase is currently being measured. The data will be interpreted after thorough characterization of the anatase solid. These preliminary results would imply that the inorganic nanomaterials may have a much stronger affect on the distribution of inorganic pollutants than carbon-based nanomaterials.

In the course of these investigations, it was also noted that particulate surfaces can cause precipitation of salts out of solution. Such an effect has not only significant implications for environmental processes, but it also has tremendous potential in industrial applications. We have studied the effect of anatase on the nucleation rate of BaSO₄. BaSO₄ is a common natural mineral and it is also one of the common scaling minerals in both water treatment facilities and oil and gas production system. Preliminary results on the precipitation of Ba from solution versus time in the presence and absence of anatase illustrates that anatase enhances BaSO₄ precipitation significantly. It is anticipated that the anatase nanoparticles will be even more efficient at removing BaSO₄ and other salts from solution by virtue of their high surface area. For example, it is estimated that the anatase particles used in these experiments are 400 nm in diameter; truly nanosized particles, with 5 nm diameter, might produce the same effect with 6,400 times less material. Colvin's research group is currently developing processes to produce large quantities of nanosized anatase to test these ideas in Tomson’s laboratory.

Over the next year this work will be expanded upon to include new materials (single walled carbon nanotubes), as well as a wider variety of sorbents (Tomson, Colvin, Smalley). After initially studying the impact of nanoparticles on the homogeneous solution chemistry of pollutants, selected characterized model colloids, sediments and soils will be added to experimental systems to determine if the reactivity of the nanoparticles has been altered. Environmental contaminants will include representative hydrophobic organic compounds, ionic and nonionic surfactants, cations of common heavy metals, and the anions of phosphate and arsenic (III & V). Compound analyses in the solid and solution fractions will be done via established techniques (GC, ICP, etc.). Solids will be separated by (ultra)-centrifugation, membrane filtration and HPLC and examination will be done with SEM, TEM, and AFM. The results of such studies will be combined with the results from Wiesner’s transport measurements to evaluate the potential role nanoparticles may have in facilitated transport of pollutants.

![Figure 5.3.4 Sorption of naphthalene to buckminsterfullerene and soil.](image1)

![Figure 5.3.5 Sorption of Cadmium to TiO₂ anatase.](image2)
In addition, Colvin will design nanoparticles with specific strong interactions with contaminants as homogeneous sorbents. Interaction of pollutants with larger sub-micron particles has been studied in great detail over the last decade; however, many features of nanoparticles suggest that their participation in environmentally relevant reactions may be advantageous for intentionally sorbing materials. First, their small size confers greater diffusive transport and large surface area per mass for greater solution phase exposure. Also, in nanoparticles the spatial scale of ionic interactions is similar to that of the particle dimension which may optimize surface-contaminant interactions. Most importantly, the surface of the nanostructures of interest here differs significantly from polycrystalline colloidal particles. In particular, both nanocrystals as well as carbon nanotubes are single crystals which, while possessing high surface area, have few crystalline defects. All of these factors can be manipulated to enhance nanoparticle interactions with pollutants in a homogeneous solution. Once associated, nanoparticles can be separated using filtration or sedimentation processes (Section 5.3.1) thereby allowing for effective clean-up of contaminated materials.

In the next year, these sorption/desorption studies will be augmented by efforts in Wiesner’s laboratory to measure the mobility and transport of nanoparticles in porous media. Silica nanoparticles and carbon nanotubes will be introduced under controlled conditions to porous media. Transport and surface chemistry effects will be separated and used as a basis for characterizing the surface properties of nanoparticles as they are modified by material commonly present in natural waters including bio-polymers. In addition, an undergraduate project will address the environmental impacts of a growing nanochemistry industry as extrapolated from current procedures for producing nanomaterials.
5.4 Theme 4: Nanomanufacturing Facility

Theme Leader: Vicki Colvin
Personnel: 3 Faculty; 2 Undergraduate Students; 1 Postdocs; 1 Other Personnel

<table>
<thead>
<tr>
<th>Project</th>
<th>Leader</th>
<th>Investigators</th>
<th>Disciplines Involved</th>
<th>Number of Students and Post-docs</th>
<th>Current Year Budget</th>
<th>Proposed Budget</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nanomanufacturing Facility</td>
<td>Vicki Colvin</td>
<td>Vicki Colvin (Chemistry), Matteo Pasquali and Michael Wong (Chemical Engineering)</td>
<td>Chemistry, Chem. Engineering</td>
<td>1 Technician, 1 Post-doc, 2 Undergraduates</td>
<td>$240,116</td>
<td>$264,402</td>
</tr>
</tbody>
</table>

Investigators: Colvin, Pasquali, Wong

One of the most formidable roadblocks that academic researchers face in transferring nanotechnologies to commercial users is the production of large amounts (> 10 grams) of high-quality nanomaterials for systems-level testing. Laboratory reactions for nanomaterials rarely have been designed with manufacturing concerns in mind. While such processes can produce enough material for isolated technology demonstrations, they are usually impossible to scale-up to kilogram quantities without fundamental changes in chemical strategy. The academic community is generally not interested in solving what is perceived as pedestrian scale-up problems, thus most researchers do not aggressively pursue solutions to manufacturing problems. Without such tests, non-academic partners are reluctant to invest in costly manufacturing programs. This leaves most nanotechnology research stuck at the proof-of-concept stage. The aim of this project area is to introduce a new paradigm for academic and industrial collaboration that will address this serious roadblock to nanotechnology development.

Our concept is to create a nanomanufacturing facility which supports both with people and space center members who wish to explore new strategies in nanomaterial scale-up. Rather than simply complete the same processes on a larger scale, this resource is targeted to encourage researchers to rethink their approaches to specific nanomaterial synthesis. In spirit this facility is similar to academic lithographic nanofabrication facilities in that it will be staffed by full-time professionals and available as a resource to all center members. This facility was originally planned as one component of an extensive program in systems-level testing; because of the 37% reduction in our budget, however, we cancelled all systems-level testing and testbed projects. We retained the nanomanufacturing facility in our final budget due to the very positive feedback from the final panel review for this initiative. While not located in the three theme areas, we feel this issue is central to any technology transfer activities and thus an important element of our strategic plan. We have secured space for this facility in the chemical engineering department, and begun planning for the first nanomanufacturing projects. Described in brief below, these aim to develop continuous flow techniques for nanoparticle production in liquids.

The dominant paradigm in nanoparticle formation is a liquid phase batch reaction; unlike gas phase reactions to form nanoparticles, liquid phase reactions produce smaller (d < 10 nm) materials that are well passivated and unaggregated. Indeed, the highest quality semiconductor, metal and ceramic nanoparticles in terms of size distribution and surface passivation are all products of batch reactions in liquids. While these processes have been optimized to produce highly perfect and single-sized clusters, their yields are very low and typically range from 10-
100 mg of material for every 20 ml of solvent used. These low concentrations are important to limit particle growth and aggregation, yet clearly batch reactions for production are not tenable if tens of grams of materials are required.

In our first nanomanufacturing project we will adapt these reactions for nanoparticle formation to a continuous flow system. Here, reactants are mixed quickly to form nuclei, which grow during flow, resulting in particles that are separated from the reaction media through filtration or chromatography. In such a system, solvents can be recycled, leading to lower costs and environmental impact, and since particle growth occurs continuously larger amounts of material can be produced. To evaluate this concept we have chosen two model systems, semiconductor and gold nanocrystals, where the nucleation and growth processes have been studied in some detail. Since separation of particles from the liquid phase is an important and relatively unexplored issue in nanochemistry, over the last few months we have applied chromatography to nanoparticle separations (Colvin). Nanoparticle size separation would provide an additional processing capability in the mass production of monodisperse nanoparticles. We have shown that gold nanocrystals of different size can be separated by size exclusion chromatography; in addition, particles of the same size but coated with different chain length alkyl groups can also be separated. Further studies of the batch reactions to determine the particle growth rates as a function of reactant concentrations and temperature (Colvin, Wong) will be completed. Such data will be used in simulations of the flow fields in various candidate mixer/reactor designs to predict particle size distributions and yields (Pasquali). For example, the use of microchannels may be advantageous as a reactor design concept by confining nanoparticle nucleation and growth to controlled temperature and velocity zones. This simulation data will be used to construct liquid flow reactors which will allow for continuous processing of nanoparticles (Wong).

This nanomanufacturing facility is an important component of our industrial outreach strategy. We will develop a Nanomanufacturing Consortium of industrial and government partners with experience in specialty chemical manufacturing and an interest in becoming suppliers for this exciting new market. Many of the most logical partners are existing startup ventures established by center members, such as Carbon Nanotechnologies, Inc. (Smalley), Nanospectra (Halas/West), and Nanotec Filtration (Barron/Wiesner/Colvin), some of which are already grappling with fabrication issues. Companies such as Dow, EMI Industries, and ATMI have expertise in chemical manufacturing and a strong interest in positioning themselves in this area. These industrial manufacturing partners will receive from the center access to the technical reports from the nanochemistry facility, favorable treatment should intellectual property be licensed or developed, access to industrial affiliate companies who are developing nanotechnology applications and use of the nanoshare instrumentation facility. We will also encourage visiting scientists from industry to spend six months to a year in this facility learning the techniques for nanomaterials fabrication. The outcome of these projects will be materials available for development projects, as well as technical reports detailing experience gained in reaction optimization and scale-up.

This project also may figure into an educational outreach program with Hochschule Bremerhaven University of Applied Sciences. We are exploring the possibility of hosting two of their Masters-level students per year for six months to attend classes at Rice and work in the
nanomanufacturing facility. Implementing this outreach project is contingent upon acquiring external funding to support the students.
6. Education and Human Resources

In order for nanotechnology to have the impact upon society that we envision a new workforce must be cultivated, one experienced with nanoscience and nanoengineering. This is a challenge for our outreach program at many levels. Because of nanotechnology’s young age, the general public, which includes parents and teachers, understand little about its great potential for society and are less likely to recommend it as a subject for study. Declining enrollments of science and engineering majors at the college level limit the number of enthusiastic, diverse students willing to enter graduate programs of any type. Finally, the interdisciplinary nature of nanotechnology presents a challenge for graduate education organized around traditional departmental boundaries. Our outreach efforts address these issues directly in a series of programs aimed at K-12 teachers, college and graduate students, nanotechnology researchers, business leaders, and ultimately the general public.

In all of these, we exploit the capacity that nanotechnology has to spark a sense of wonder in students and adults alike. We believe that, like the space program, the nanotechnology initiative holds the potential to catalyze public interest in all types of science and technology. At the K-12 level, we train teachers to use nanotechnology as a springboard for teaching general science, and we reach into the elementary school level with the engaging imagery of NanoKids™. At the undergraduate level and beyond, our emphasis shifts to introducing nanotechnology-specific course material into the curriculum and to preparing students for nanotechnology related careers in both academia and business. We partner with other organizations on the Rice campus to reach out to the largely untapped reserves of minority students that might otherwise seek alternate careers or bypass higher education altogether. Finally, we recognize the value an informed public has for our emerging technology, and work to develop accessible stories about nanotechnology and society for a public lecture series.

6.1 K-12 Programs

Our centerpiece educational outreach program focuses on ninth grade science teachers. We feel that by investing in high quality, long-term teacher training, we can multiply our center’s investment many times over as our teacher alumni will inspire not only generations of students, but also their peers as well. We intentionally targeted the ninth grade teachers, rather than the more sophisticated and educated advanced placement teachers, because of the central role that ninth grade science plays in the Houston Independent School District (HISD). Along with algebra, failure to pass ninth grade science is a major reason many students in the HISD do not advance past 9th grade. In Texas this class is an integrated physics and chemistry course (IPC) that is often the first assignment given to young teachers who may not have extensive scientific training, yet are expected to succeed if they want to advance to courses that are more "desirable". Quite often, the teachers want to improve but have no mechanism within their schools for getting help. These teacher-centered challenges are exacerbated by those faced by their students. Not surprisingly, there is a drastic dropout rate in high school; statistics from the United States Department of Education show that only 47% of those HISD students who entered 9th grade in 1994 graduated in 1998. As in most other large urban school districts, many HISD students face serious barriers to learning, including poverty (75.4% of students are on free/reduced lunch), migrancy (38.2% mobility rate), and language (26.5% have limited English proficiency). Additionally, investing our efforts in HISD impacts mostly underrepresented groups simply due
to its diverse demographic makeup: 52% Hispanic, 34% African American, 11% White, and 3% Asian. The three phases of our program are:

- **CHEM 570, Spring Content Course**: refreshes understanding of core science concepts and connects those concepts to ongoing nanotechnology research.
- **Summer Internship**: reinforces science as a process by placing teachers in research laboratories.
- **Model Science Lab II**: a semester-long sabbatical residency to introduce constructivist teaching techniques.

In addition to this professional-development series, we are implementing a number of other K-12 programs:

- **Laredo/Rice IPC Teacher Training Workshop**: An intensive 3-day workshop version of CHEM 570, presented to teachers from the Laredo, TX school districts.
- **High School Summer Academy**: A summer science-fair workshop.
- **NanoKids™ Curriculum Development**: Curricular materials using anthropomorphized molecules to draw students into the science.
- **Other Programs**: Direct contact between center members and K-12 students on an ad hoc basis.

Details concerning all of these programs follow.

### 6.1.1 CHEM 570, Spring Content Course

This two credit-hour course offered in the evenings has the dual goals of refreshing the teachers’ understanding of core physics and chemistry concepts, and connecting those core scientific concepts to ongoing nanotechnology research. For the first hour of each evening, basic science concepts are reviewed and extended through the use of a modified socratic method approach, providing a solid foundation of understanding that the teachers can draw upon in their classes. The second half of each class period is a presentation by a center researcher on current investigations that relates to the scientific concepts discussed in the first hour.

Currently in its inaugural semester, CHEM 570 has an enrollment of fourteen teachers, 12 from HISD and 2 from the Ft. Bend school district. Through increased advertising of the course, we expect future years’ classes to reach at least twice that number.

![Figure 6.1 Dr. Kevin Ausman introducing CHEM 570 high-school teachers to the historical origins of the atomic-molecular theory.](image-url)
6.1.2 Summer Internship

We have tailored our summer program to the needs of 9th-grade Integrated Physics and Chemistry teachers. Rather than have teachers work on independent research as is generally the case for a Research Experience for Teachers (NSF-RET) program, we use the center’s resources to focus instead on techniques for translating the center’s research, both its methodology and its results, into a classroom setting. The goals of our summer internship program, to be piloted in the summer of 2002, are to strongly reinforce each teacher’s sense of science as a process, to deepen each teacher's understanding of the achievements and potential of nanoscience, and to apply lessons learned from the content class to a research setting.

We do this by asking that our summer teachers create a web page and lesson plan that explain the research of the host lab at a level appropriate for a high school teacher or student. Over the course of the four-week program teachers will spend four days per week observing and assisting in research, as well as interviewing lab personnel. On the fifth day of each week, the teachers will meet together to share and discuss activities in their respective labs, review existing nanoscience and materials science classroom resources, and develop a personal plan that applies center science to at least one unit in IPC. The teachers’ understanding of nanoscience will be demonstrated by the construction of a web page and course materials. Training in the creation of web pages will be done by the Rice User Services Training Coordinator. The web page will provide the researcher with a product of value in exchange for the time and space committed to the teacher, while the teacher will learn about the research and about web page construction.

6.1.3 Model Science Lab II

Our teacher-training program will use our unique center resources to extend a successful middle-school program to the 9th- and 10th- grades. We are fortunate here at Rice to have a teacher-training model for our new program, the Model Science Lab (MSL), which is an intense residency program in which eight middle school science teachers spend a sabbatical year in an inner city school studying and class-testing discovery-based approaches to science education. Tangible achievements of the MSL include an almost perfect teacher retention rate (95% after 11 years), the professionalization of a cadre of teachers who act as peer mentors, and the improvement in student test scores. The students of MSL teachers demonstrated greater improvement on both the state achievement test and on a pre/post modified NAEP (National Assessment of Educational Progress) test than students taught by control teachers in each of their schools.

![Figure 6.2 Lanier Middle School Model Science Lab students exploring electric circuits](image_url)
The Model Science Lab II, our 9th/10th-grade successor program to this successful 5th-8th-grade program, will be piloted in the fall of 2002 with four teachers, three funded by our center and the fourth and the programmatic costs funded by the Cain Foundation. The four teachers for this pilot will be selected from the participants in the summer internship program described above. In future years, further external funding will be sought to increase the complement of teachers to eight.

6.1.4 Laredo/Rice IPC Teacher Training Workshop
Leveraging the curriculum developed for CHEM 570, described above, the center is developing an intensive 3-day workshop covering the same material to be held in June for a set of 9th-grade IPC teachers from Laredo, TX. Even more than HISD, the Laredo school district’s students suffer from serious barriers to learning (91.4% were categorized as economically disadvantaged in 2000), and since the district is located 160 miles from the nearest major metropolitan area, its teachers have only limited access to professional development opportunities. In addition to running the workshop, the center will cover the travel expenses for approximately fifteen teachers to participate in the event. Additionally, the center’s efforts will be strongly targeting traditionally underrepresented minorities (99% of the district’s student population is Hispanic).

6.1.5 High-School Summer Academy
Science fair projects provide an excellent tool for discovery-based pedagogy at the high school level. Further, the excitement and interest that can be generated in students by new, vibrant fields such as nanotechnology can dramatically increase the effectiveness of such a teaching tool. We will use the cadre of informed and motivated teachers from the HISD professional development series to draw high school students from underrepresented groups into the research activities of the center. This process will begin with a 1-2 week Science Academy for promising 9th/10th grade students identified by MSL teachers. Structuring the Academy as a science fair workshop in which students learn how to construct and test a hypothesis will allow the process of scientific inquiry begun in the MSL intern's classroom to continue. At this age, students are at a pivotal time in the evolution of their career planning. If we can continue to excite them about the process of scientific discovery, more of them may consider studying science and engineering in college. Promising graduates of the Academy will be invited back in subsequent summers to work in the research labs as assistants or on their own science fair projects under the mentorship of a center researcher. The impact of student involvement in center activities will be assessed through student interviews or surveys. Each student's progress through high school and beyond will be tracked for the duration of the research grant. The center will coordinate activities and work aggressively with Rice's Coordinator of Minority Recruitment; their staff has been drawn from backgrounds similar to those of the minority students we are targeting, and their mentorship will be important in developing minority student relationships.

6.1.6 Nanokids™ Curriculum Development
Center member James Tour has synthesized organic molecules whose structures are visually reminiscent of children. The NanoKids™ program, partially supported by center funds, is developing curricular materials around animated characters based on these molecules (see figure 6.3). These anthropomorphic molecules inherently contain a visual concept that utilizes universally recognized forms exhibiting human characteristics that can be tapped to instruct,
motivate, and entertain students. The program is initially targeting the middle-school level, as that is the point in the normal science curriculum where the concept of molecules is introduced. A series of modules are under development, consisting of animated video/DVD stand-alone lessons and interactive CD workbooks with appropriate experiments, field trips and ancillary activities. A teacher's study guide and a parents' study guide will accompany each module, so that learning nanoscale science becomes a school and family affair.

Formative evaluation is key to the NanoKids™ development process, and is in full swing through student, parent and teacher focus groups. Basic science teaching and learning techniques, character looks and qualities, interest-catching settings, and prospective music styles are under scrutiny by experts in the field and by those whom the project is meant to serve. Spending the time up front to determine preferences and needs will enable us to produce an itemized outline of the completed series for the first target group and the first completed script with storyboards, music and science support data by May 30, 2002. The high-school teachers taking CHEM 570 will serve as a focus group to review and evaluate development concepts, and there will be an opportunity for one or more of the teachers participating in the summer internship program described above to work intensely on this project.

6.1.7 Other Activities

**Activity:** College Awareness Day, McReynolds Middle School  
**Led by:** Dr. Kevin Ausman  
**Intended Audience:** A sixth-grade class at McReynolds Middle School, Houston, TX  
**Approximate Number of Attendees:** 30  
**Narrative:** Delivered a presentation entitled, “Nanotechnology: How the Science of the Very Small will Change the World,” in an effort to spark an interest in attending college among a group of at-risk students.

**Activity:** Laboratory visit by students from Kinkaid High School, Houston, TX  
**Led by:** Prof. Andrew Barron  
**Intended Audience:** High school science students  
**Approximate Number of Attendees:** 30
Narrative: Arranged a tour of the laboratories. Students were shown how chemists handle air sensitive compounds and liquid nitrogen.

Activity: Owlchemy presentation for National Chemistry Week
Led by: Prof. Andrew Barron
Intended Audience: Undergraduate students
Approximate Number of Attendees: 35
Narrative: A discussion of the types of interesting projects a chemist can become involved in, including such diverse possibilities as book preservation at the Library of Congress and the Fire Department’s Hazardous Materials teams, leading into a story about being involved in a murder trial as an expert witness.

Activity: NSF GK-12 Fellows Program Presentation
Led by: Vicki Colvin
Intended Audience: HISD middle and high school teachers and GK-12 fellows
Approximate Number of Attendees: 35
Narrative: A welcome presentation was made by Fellows Program Coordinator, Julie Overlease, followed by presentations from 3 groups of fellows, where attendees rotated to each of three presentations. Finally, Vicki Colvin presented, “Nanotechnology: From Science Fiction to Science Fact,” to all attendees.

6.2 Undergraduate Programs
Our undergraduate educational development programs encompass a Minority Research Experience for Undergraduates program, new course development, and modification of existing courses.

6.2.1 MREU Program
Involving students in discovery-based scientific inquiry is the primary objective of our Minority Research Experience for Undergraduates (MREU) program, to be first offered in the summer of 2003. This program is modeled after an existing REU program offered by the Rice Quantum Institute, in which undergraduates work on independent research projects in a Rice lab for 10 weeks and present their work at a conference held at the end of the summer. Our MREU program will specifically target students from regional colleges and universities with diverse populations through faculty recruitment trips. It is possible for advanced high school students from the Academy or MSL teacher's classes to participate in this program. In addition to providing a research experience, we will have weekly social events in which students can interact with one another and discuss any issues of importance to them regarding their career plans.

This MREU program will be coordinated with Rice’s existing, exceptionally successful Alliances for Graduate Education and the Professoriate (AGEP) program. In particular, the AGEP summer undergraduate research program is specifically designed to give hands-on research experience to undergraduate students in the fields of math, engineering, science, and technology-related disciplines. This AGEP program is itself the successor of a highly effective Spend a Summer with a Scientist (SaS) program, which over its lifetime demonstrated an impressive 62% enrollment of its undergraduate participants, of whom 88% were Hispanic or African American, in graduate school. For comparison, less than 9% of Hispanics and African
Americans who received baccalaureate degrees entered graduate school over the same period, according to National Center for Educational Statistic; the percentage is even lower in the specific fields covered by Rice’s SaS program.

6.2.2 New Undergraduate Courses under Development
For graduate and undergraduate education, CBEN’s vision is to create a series of interlocking courses in nanoscience and education. The planning for the start of this curriculum is already underway, and will leverage two new programs at Rice. One of these, the Sloan Professional Master’s program, has majors in Nanotechnology (physics) and Environmental Decision Making. The second, the Rice Connexions program to develop web-based materials, started in the Electrical Engineering department, provides staff and a web programming language well-suited for equation display and self-study. Many of the courses described in this section are also available to graduate students, and many of the courses described in the graduate section are also available to undergraduates.

The Chemistry Department at Rice currently offers its upper-division undergraduate lab courses in the format of half-semester or semester themed modules that integrate skills traditionally developed in separate courses. This format is intended to more closely simulate the systems-level focus that underlies many research projects, especially those span traditional divisions within a discipline. In an example of a current module, students synthesize, separate, and characterize fullerenes using electrochemical and photophysical techniques, thus integrating skills conventionally within the separate domains of organic, analytical, and physical chemistry laboratories. We are planning a semester module in environmental waste remediation using nanoscale titania for the spring of 2003. Drs. Mason, Barron, and Wiesner will use the photooxidation of organic halides by nanoscale titania as a case study in the cost-benefit analysis of clean-up strategies for environmental science. This new course will be disseminated to the education community at national meetings such as Biennial Conference on Chemical Education and through publication in journals such as the *Journal of Chemical Education*.

6.2.3 Undergraduate Courses Modified
Several pre-existing Rice University courses have been modified to include center research. In addition, some graduate level classes, described below, are available for advanced undergraduates. These modified undergraduate courses include:

- **BIOE 441: Advanced Bioengineering Laboratory.** This course is required of all seniors majoring in bioengineering. We are currently developing a module where students will use metal nanoshells and their associated photothermal phenomena to induce tissue welding. Students will learn about the nanostructured materials and optical interactions, and then will also use this as an opportunity to use their skills in biomechanics to evaluate the efficacy of nanoparticle-assisted laser tissue welding.
- **ENVI 401: Introduction to Environmental Chemistry.** Results of CBEN research included as appropriate examples of concepts discussed in class.

6.3 Graduate Programs
Our graduate educational development programs encompass new course development, modifications of existing courses, development of an entrepreneurship education program, and outreach to Bremerhaven University of Applied Sciences.
6.3.1 New Graduate Courses under Development

There are very few interdisciplinary courses in nanoscience offered by universities at the graduate level. We feel the need for graduate education in this area is particularly pressing given our mission of integrating nanoscience into the larger research community. CBEN, working in conjunction with the Sloan Nanotechnology Physics program, is planning a two-semester lecture course in nanomaterials and nanoscience that will be team taught by several faculty, including Drs. Colvin, Natelson, and Hafner. This course will consist of interlocking modules covering topics in chemistry, physics, and materials science. This lecture course, to be augmented by materials developed with the Rice Connexions program, will be offered in the fall of 2002. Ultimately, we will produce a textbook and interactive web page that will serve as a resource for courses at other institutions. A two-semester course on nanostructures and nanotechnology, exploring the physics of structures and devices at the nanometer scale, is under development (Natelson), as is a two-semester course in experimental techniques for physics (Hafner). Also planned is a new graduate-level course in microscopy of nanostructures (Stemmer). Non-center faculty Alex Rimberg is developing a course on characterization and fabrication at the nanoscale. A seminar course covering recent advances in nanoscale science and engineering is planned for 2004. In addition, interactive light propagation software designed for use in courses in biomedical optics will be developed and tested at Rice and then broadly disseminated to the optics community (Drezek). The software will allow students to explore (1) relationships between subcellular biochemical and morphological structure and light scattering using a three-dimensional FDTD model, and (2) relationships between tissue optical properties, fiber optic delivery and collection geometries, and remitted reflectance and fluorescence signals using a Monte Carlo model.

6.3.2 Entrepreneurship Education

An important element of our strategic plan is the realization that in the future many of the most important industrial collaborations our center members will engage in will involve small startup companies. Not only are they becoming a major employer of technical PhDs, but these businesses are also becoming the route by which high-risk technologies are developed. These trends are due in part to the bull market of the mid- to late 1990's; however, a principle that has withstood the test of time is that breakthrough technology is best developed by small groups of highly skilled, risk-taking individuals. These companies, which often involve the inventors as owners and partners, have very different concerns than larger corporations and require much more active involvement of inventors. Our entrepreneurship education programs are designed to prepare our students for these job opportunities and to forge strong relationships between the center and those corporations founded by our own members.

The entrepreneurial model for business development requires that inventors have access to the resources and talent of the business community. This clearly requires that academics have many opportunities to interact with business professionals, ideally in a forum to present their inventions. We are implementing collaboration between the center and the Jones Graduate School of Management to expand on a program that fosters this interaction. The Rice Alliance for Technology and Entrepreneurship is the centerpiece of the University's bold initiative that joins the resources of the Wiess School of Natural Sciences, Brown School of Engineering, and Jones Graduate School of Management together with other academic units and the Office of Technology Transfer. The mission of the Rice Alliance is to promote collaboration among
university researchers and technology entrepreneurs, the outcome of which is the formation of new technology firms that bring to the marketplace innovative and useful products and services. In addition to the educational activities described below, our center is collaborating with the Rice Alliance on an annual Innovation Concept Forum, described in section 7 of this report.

**Entrepreneurship Education Workshop.** To start new companies, or to interact with existing startups, academic inventors must also have a rudimentary knowledge of business practices and language. We will hold a two-day workshop in Entrepreneurship Education for Researchers for professors, post-docs, and graduate students. This course on the commercialization of research discoveries in science and engineering will be staffed by professors in Rice’s Jones Graduate School of Management and industry participants (e.g., local entrepreneurs and investors) involved in the Rice Alliance or as industrial affiliates. The center will sponsor the attendance of its own members and promising junior nanoscience researchers at other academic institutions. Topics to be covered in this course will include intellectual property, evaluation of business plans, negotiation skills, corporate governance in new ventures, common mistakes of entrepreneurs, and university incubators. The first of these workshops will be held in conjunction with our first annual conference, in the fall of 2002.

**Graduate Course in Entrepreneurship for Scientists and Engineers.** In keeping with our focus on creating technical Ph.D.s well informed about career options, as well as our mission to enhance our member's knowledge of business practices, we offer a year-long graduate course entitled "Entrepreneurship for Scientists and Engineers" which is co-taught by center faculty from the science, engineering and management schools. This class has already been developed for chemistry students with the support of the Coleman and Dreyfus Foundations. First semester topics include: venture financing, intellectual property (IP), market research and organization behavior. In the 2nd semester, science and management students will work together in teams to perform extensive market and IP research for one or more center inventions, culminating in the creation of a business plan for commercializing a center innovation. Twenty-nine students participated in the first semester of this course in 2001, and nine are participating in the second semester in 2002.

**6.3.3 Graduate Courses Modified**
Several pre-existing Rice University courses have been modified to include center research. These include:

- **BIOE 531: Biomaterials Engineering.** A module has been added to this course focusing on nanostructured materials.
- **BIOE 572: Fundamentals of Systems Physiology.** A new semester project has been added in which students advise a mock venture capital firm about potential investments in novel bioengineering technology. Nanoengineered optical contrast agents are used as the sample technology in class.
- **CENG 603: Rheology.** Results of CBEN research included as appropriate examples of concepts discussed in class.
- **CEVE 534: Transport Phenomena and Environmental Modeling.** Examples illustrating transport of nanoparticles in the environment have been introduced.
- **ENVI 550: Applied Water Chemistry.** Results of CBEN research included as appropriate examples of concepts discussed in class.
- **ENVI 635: Advanced Topics in Water.** Results of CBEN research included as appropriate examples of concepts discussed in class.
- **MGMT 750/CHEM750/MSCI 750: Entrepreneurial Management for Science and Engineering.** Results of CBEN research included as appropriate examples of concepts discussed in class.
- **MGMT 751/CHEM 751/MSCI 751: New Venture Creation for Science and Engineering.** Results of CBEN research included as appropriate examples of concepts discussed in class.

### 6.3.4 Hochschule Bremerhaven University of Applied Sciences

A partnership with Hochschule Bremerhaven in Bremerhaven, Germany, is being explored, wherein two Masters-level students per year would visit Rice for six months to take classes and work on projects in the center’s nanomanufacturing facility. This would help fulfill their degree requirements, and will provide extra applied-sciences help in scaling up nanomaterial syntheses. Implementing this outreach project is contingent upon acquiring external funding to support the students.

### 6.4 Community Programs

Many of our center's members are already involved in bringing the excitement of nanoscience to the public through a "Frontiers of Science" course offered by the School of Continuing Studies. This eight-week lecture course has been enormously popular with enrollments exceeding 80 attendees. In Y02 of this grant, our center will provide speakers and materials to continue and expand this very successful program.

### 6.5 Diversity

Many of our core programs have been designed specifically to target traditionally underrepresented minorities. These are:

- **MREU Program:** Minority undergraduates are specifically recruited into this program. We will augment the efforts of Rice’s very successful AGEP program.
- **3-Phase Professional Development Series:** This series, comprised of CHEM 570, the summer internship, and the Model Science Lab II, targets teachers from the Houston Independent School District (HISD). The HISD student population is highly minority based: 52% Hispanic, 34% African American, 11% White, and 3% Asian.
- **Laredo/Rice IPC Teacher-Training Workshop:** The teachers to be included in this program teach in the Laredo school district, which has heavy minority representation: 99% Hispanic, 1% White.
7. Outreach and Knowledge Transfer

7.1 Nanotechnology and Environment Workshop
CBEN and the Rice Environmental & Energy Systems Institute (EESI) organized a two-day workshop to launch the environmental nanotechnology research thrust of the center, held on December 10-11, 2001. Funding for the workshop was obtained from the French Embassy to bring together Rice scholars and French researchers from the Centre Européen de Recherche et d’Enseignement de Géosciences de l’Environnement (CEREGE). The first day attracted over 80 participants to public presentations exploring the range of nanomaterials currently being created, their possible applications to improving environmental quality, and their potential dangers as environmental pollutants. The second day consisted of closed-door discussions on new directions for collaborative investigations, from which a research needs document will be published. The event received excellent coverage in the Houston and French press. A follow-up workshop that will bring Rice researchers to France in 2002 has been proposed by the French Embassy.

7.2 Annual Conference
The center will host a yearly conference with research talks and posters, tutorials/workshops for graduate students and industrial scientists, and social events to bring together faculty, students and industrial scientists from the nanotechnology community worldwide. We will hold this conference in conjunction with the annual meeting of our industrial advisory board so that board members may interact with as many center members as possible. This conference will be scheduled during the Rice University autumn semester mid-term recess, which this year will fall on October 14-15.

7.3 Industrial Affiliates Program
We are aggressively developing relationships with established industries through our industrial affiliates programs. This program focuses on educating industrial leaders and scientists in the basics of this new discipline and exposing them to the wide variety of center research and technology development. The aim is to identify and prepare champions of nanotechnology within established industries capable of sponsoring partnerships with center members once viable products are identified. Our program, currently under development, is loosely based on successful affiliates programs of several engineering departments at Rice. Membership fees in this program will be on a sliding scale depending on company size and these fees will be used to sponsor related activities. Membership will entitle the company to a number of benefits and programs. First, companies with particular interest in developing the techniques for nanomaterials fabrication will be encouraged to send a senior scientist to work in our nanomanufacturing facility for an extended period. Other affiliates will be encouraged to send a scientist or manager to the center for a 2-3 day visit with center members and to give a seminar on the emerging technical needs of their business. Company leaders will also be invited to the annual conference for half-day tutorials in key areas of nanoscience, lectures on center research, and social activities, designed to familiarize them with center personnel. Affiliates will be invited to appoint a member to our industrial advisory board. Companies at the higher-end of the fee schedule may have part of their funds dedicated to a graduate student fellowship, named for their institution. To facilitate hiring in this rapidly growing area, industrial affiliates will have access to a database of past and current center students and post-doctoral associates. Finally, affiliates
will have the services of the Executive Director of Operations, who will foster partnerships between center members and industrial affiliates. This person will visit affiliates on-site annually to learn firsthand about the business and provide updates on relevant center research.

### 7.4 Industrial Collaborations/Interactions

We are collaborating with Tnemec, Inc. and Isotron, Inc. to develop an economical approach to the production of the alumoxanes (Barron). This is being accomplished through a high shear mixing rather than the more traditional thermal processes. Initial results show promise.

### 7.5 Entrepreneurship

The mechanism by which the Rice Alliance, introduced in section 6 of this report, fosters collaboration is the “Innovation Concept Forum,” which convenes students, faculty, alumni, technology entrepreneurs, and members of the business community as collaborators on new business ideas based on scientific research at Rice. Sixty-three science- and engineering-based business concepts have been presented at Forum events held from October 1999 to January 2001—some of these new ventures already have received national attention and many of them have been funded by investors. The Rice Alliance has hosted presentations from researchers working on a wide array of nanoscale science and technology problems including carbon nanotubes, molecular electronics, metal nanoshells, and nanofiltration. The Rice Alliance has also hosted presentations by undergraduate and graduate students and Rice alumni. The Rice Alliance has expanded its efforts into the area of life sciences/biotechnology through partnerships with institutions in Texas Medical Center (located in Houston). For example, on November 18, 2000, the Alliance held a joint Forum event with M.D. Anderson Cancer Center to spotlight life sciences/biotechnology discoveries from both Rice and M.D. Anderson such as innovations in the use of nanoscale technology to treat cancer. The Rice Alliance has been a successful vehicle for outreach between the University and the business community. One Alliance presenter, Todd Litton (Rice graduate student) stated: “We envisioned that it would be all academics but there were a lot of business people. The great thing about the Alliance is that it’s really geared to making good ideas commercially viable.” Our center is building on this strong foundation by sponsoring annual Innovation Concept Forums dedicated to promoting the inventions of nanoscience researchers, the first of which is to be held on March 1, 2002.

### 7.6 Presentations/Other Outreach

#### 7.6.1 Research Presentations


### 7.6.2 General CBEN Outreach

K. Ausman attended the U.S./Germany Joint Meeting on Nanoscale Science and Engineering at the Massachusetts Institute of Technology on December 6, 2001. Presented an overview of CBEN.


8. Shared Experimental Facilities

CBEN is committed to forming at Rice a major instrumentation facility for nanoscience and engineering. Over one million dollars of funding provides for new equipment for CBEN, and much of that is to be acquired in year 1. These purchases will add to an already extensive nanoequipment portfolio paid for from a five million dollar alumni fundraising campaign completed by Rice’s Center for Nanoscale Science and Technology in 1996. To take full advantage of this extensive investment in nanotechnology instrumentation, however, requires a management strategy which provides for long-term stewardship of the equipment. Over the past several months CBEN has put into place the elements of what we believe will be a robust and lasting solution to the problem of shared equipment management. The highlights of our program include:

- **Strategic equipment purchases**, to supplement existing instrumentation.
- **A campus initiative** for faculty management called the shared equipment authority.
- **New technical staff positions** for training and maintenance.

### 8.1 Existing equipment

Rice University has laid the groundwork for our center’s experimental facilities as part of their three-year fundraising campaign for nanoscience. Our new nanoscience and technology building, Dell Butcher Hall, houses a state-of-the-art equipment room designed for minimal vibration and electrical isolation. It is now only 30% occupied by common equipment acquired through fundraising campaigns and collaborative instrument grants. This equipment includes a Phillips environmental SEM, a JEOL electron beam lithography system, two Digital Instruments Atomic Force Microscopes, an Omicron low temperature UHV-STM, and a variety of smaller items such as sputter and spin coaters. Other instrumentation located elsewhere on campus and available for common use include a JEOL 2010cx transmission electron microscope, a Nicolet FTIR microscope, a high-resolution X-ray diffractometer and an ISA Raman microscope. Additionally, the Texas Center for X-ray Crystallography is housed at Rice and manages two single-crystal, a powder, and a small-angle X-ray diffractometer.

### 8.2 Strategic equipment purchases

$1.3M of internal cost-sharing funds has been promised for equipment purchases for CBEN, $750,000 of which were made available in Y01. $330,000 has been authorized for a new scanning electron microscope to allow for the imaging of biological materials, as well as the mesostructure of nanofiltration and bone replacement polymers. $100,000 will be used within the next month to upgrade our ten year-old transmission electron microscope. While this instrument is capable of high resolution imaging, its reliance on film for imaging and the lack of a TV-rate camera for on-screen astigmatism adjustment make it difficult to use for quantitative high-resolution microscopy. This upgrade will retrofit the microscope with a digital camera and software for routine high-resolution imaging. $450,000 is earmarked for the acquisition of a parallel supercomputer with multiprocessor nodes running in shared-memory SEP configuration through high-speed switches. Most of the parallel machines at Rice are obsolete or dedicated to specific groups. This facility will support both the memory applications (e.g. the PDE codes of Pasquali and Zygourakis), and the massively-parallel MPI codes (e.g. the molecular dynamics codes of Ma and Yakobson and the quantum mechanical simulations of Scuseria and Yakobson).
The balance of roughly $400,000 will be allocated in year 02 in order to respond to the quickly changing needs of new projects.

### 8.3 Campus Initiative in Equipment Management: The SEA

Maintaining expensive equipment whose users are widely distributed across departments is a serious organizational challenge. Previously at Rice, equipment has been used primarily within a department, and the departments have been individually responsible for identifying appropriate sources of funding for maintenance costs, including user fees when the equipment is used for more than one research project. As stated in the original proposal, CBEN recognized that a shared instrumentation stewardship program would greatly benefit multi-departmental users of expensive scientific instruments. To this end, the **Shared Equipment Authority** (SEA) has been formed.

CBEN played a lead role in the formation of this faculty initiative. The deans of natural sciences and engineering have agreed to transfer control of such shared equipment, roughly twenty instruments across campus, to the SEA faculty oversight committee. Chaired by the co-director of CBEN, Dr. Vicki Colvin, this faculty working group provides a forum for setting instrument policies, user fees, and debating resource allocations. Fees will be assessed to all users in accordance with established university policy and procedures for user fees. All CBEN equipment will serve the faculty community and CBEN researchers through this organization. While SEA is a CBEN initiative, its membership is not limited to CBEN participants. This is because a long-term solution to the problems of shared equipment infrastructure cannot be developed by considering only those instruments purchased by single centers (like CBEN) or single departments.

CBEN will provide a central organization for implementing the policies and user fees outlined by the SEA. Center staff administer all existing equipment relevant to CBEN activities as well as new equipment purchased by the center. One important goal of this administration is to develop web-based management tools by the end of 2002. Web-based guides to the center’s equipment with on-line manuals, sign-up sheets, and checkout protocols would be enormously useful and efficient. The SEA web page currently being designed is the first step toward a web-based user accounting system.

An important issue for this organization is the strategy for cost recovery. Our vision for the SEA is that within five years it will be a financially self-sufficient organization; SEA analysis of past usage patterns and projected expenses, however, suggests that user fees can only provide 20-30% of instrument costs. This is due both to the relatively small size of the Rice faculty, which leads to few billing hours relative to larger state schools, as well as the rising costs of maintenance contracts for large equipment such as electron microscopes. The Rice administration is committed to maintaining the technical staff positions after the funding cycle of the center, with the remaining expenses to be funded through user fees and other sources. A long-term solution, however, requires a substantial increase in revenue for the SEA, the goal of two new SEA programs.

The first is the acquisition of non-federal monies for instrument stewardship. CBEN is working now with Rice’s Office for Development to identify individuals and private foundations who
would be willing to donate money for these purposes; the presence of a NSF center at Rice in nanotechnology is good leverage for this type of fundraising, and many of the same people who contributed to the highly successful nanocampaign in 1996 are being approached again. We hope to secure funds from these sources, and develop a modest endowed fund to support SEA activities.

The second program aims to increase the usage of all SEA instruments through training sessions that recognize the needs of ‘exploratory’ users. Often in nanotechnology research, researchers bring several tools to bear on a single problem, and will explore many instruments in order to find out which ones really answer the important questions. To address the needs of such users, we are designing weekend workshops which illustrate how key instruments may be used to solve problems in certain disciplines. For example, Hafner will lead ‘Atomic Force Microscopy in Biology and Bioengineering’. A key component of this workshop is the time set aside for participants to evaluate their own samples under the supervision of experienced users of AFM, with the hopes that they will become regular users of the technique. Similar workshops in electron microscopy (Stemmer), FTIR and Raman microscopy (Wong), and confocal methods will also be developed. It is our intention that these workshops will motivate researchers to invest time in the training required to become independent and successful users. If instrument use can be doubled, then cost recovery through user fees will contribute to a larger fraction of maintenance costs.

8.4 Full-time staff for student training and equipment maintenance.

Two permanent, full-time technical staff positions to oversee experimental equipment are allocated for Y01 funding. As discussed in the management section (9) one full-time staff person maintains microscopes while the second is available for biological instrumentation, primarily NMR. These staffers will share responsibility for instrument maintenance, serve as the contact point for repairs, and offer training to students, post-doctoral associates, and visiting scientists. The microscopist will offer three half-semester, hands-on lab modules focusing on practical skills to complement a new graduate-level course in microscopy of nanostructures (Stemmer). In this formal environment, students can focus exclusively on mastering machine usage before applying the instrumental methods to innovative research problems. Moreover, well-trained instrument users will be less prone to misusing these expensive and sensitive instruments. The system administrator will be responsible for configuring the machine, adding users, doing periodic upgrades, maintaining a web page for the facility with information on the queuing system and software manuals, and delivering periodic training seminars for new users.
9. Personnel and Management

In the past five months, CBEN has identified all but one of its full-time staff members and these personnel have begun active administration of the center’s outreach and research programs. The remaining unfilled position, currently advertised, is the PhD level technician responsible for shared microscopy equipment training and maintenance.

The center management structure and personnel remain close to what was proposed in the original grant; changes have occurred in the titles of some positions to ensure the best possible candidates were attracted to CBEN. A physical home for the center has been located between the engineering and natural science departments on the Rice campus. This 1000 square foot space has been renovated to provide desks and meeting areas for center business. Here we review our management strategy, and introduce the center staff responsible for outreach and shared equipment.

Our center management has four distinct functions. While the tasks are shared among all center participants to some extent, the primary contact for each is listed below:

- Long-term strategic planning (Director, Dr. Rick Smalley)
- Resource allocation (Co-Director, Dr. Vicki Colvin)
- Day-to-day operations (Executive Directors, Drs. Ausman and Kulinowski)
- Evaluation activities (Senior Advisor/External Advisory Board)

Dr. Rick Smalley takes primary responsibility for the long-term planning process for CBEN, which will begin this summer in a series of meetings involving both internal and external people.
One meeting will involve our senior advisor, Dr. Neal Lane, and the CBEN external advisory board. This group will develop a strategic plan for CBEN which lays out 3-5 year goals for the research and outreach activities of the center. Dr. Lane’s extensive experience as White House science advisor and the Director of NSF will provide an important perspective for our planning process. Moreover, since Dr. Lane is not directly involved in the management or research organizations of CBEN he can provide an informed yet objective perspective about the center from within Rice University. The CBEN external advisory board will help author the strategic plan. The composition of this board is being finalized during March and April, with both directors and our senior advisor active in the selection process. After 2002, annual meetings of the advisory board will ensure that the strategic plan—a 5-page document to be made available on the center web page—is continually refined and responsive to the inevitable changes in center directions.

In addition to producing a strategic plan, our long-term planning process also involves the determination of concrete measures of center performance, and lays out targets for those performance indicators. Drs. Smalley and Colvin will work with a group of interested center members to develop proposed metrics, and introduce these to the external board for evaluation. In the first year of the program, these targets will address the number of interdisciplinary projects started, publications with multiple member authorship, students co-advised by members, industrial connections established, commercial ventures started, and the impact of educational outreach programs. These quantitative goals will be balanced by more qualitative evaluations of member participation in extracurricular center activities, such as outreach and seminars, and visibility of the center in the academic and national community. The internal working group will also refine the criteria by which individual center research projects will be evaluated. Initially projects will be judged on three points: potential for high-impact results, relevance to the center mission, and probability of success, in that order.

Co-director Dr. Vicki Colvin is responsible for leading the annual resource allocation and project evaluation processes, slated to start in early 2003. Annual research project evaluation will begin by inviting existing project leaders to submit a progress report and future funding request. Before internal evaluation, the center will seek substantive critiques of the proposals from outside the center. An external review board, consisting of several members from the external advisory board and Dr. Colvin (non-voting member), will divide proposed projects into three categories: highly recommended for funding, recommended for funding, and not recommended. Great weight will be given to this external ranking in our internal review process, as such opinions will provide a fresh and unbiased opinion of the center’s research. In addition, such involvement by external reviewers prepares us for the site visit reviews administered by the NSF. Our internal review process will be governed by the internal review board, which includes Dr. Colvin, Dr. West, and Dr. Wiesner. (Drs. Smalley and Colvin will appoint theme leaders annually based on the evolution of research and faculty availability and interest) They will be responsible for rank ordering all proposals using the external review boards comments as a guideline. The outreach projects will undergo a similar internal review process, with a rank ordering and future budget requests produced through the consensus of the Executive Directors for Operations and Education. Center leadership and administration will be evaluated through annual surveys of center members, staff and participants. Once the evaluations are completed,
Dr. Vicki Colvin is responsible for the resource allocation process and final annual budget proposal.

As originally proposed, CBEN has two PhD level positions responsible for implementing center-wide programs, monitoring research activities, and all internal and external reporting activities. The Executive Director for Education has responsibility for all educational and policy programming for the center. In addition, this position also serves as the center’s communication director, translating center findings to the media and public at large. Dr. Kristen Kulinowski has been offered this position which she plans to assume in the summer of 2002. We would like to emphasize that our naming a staff member for center education does not reflect a lack of commitment to these outreach programs. All center faculty are required to make significant annual contributions to educational efforts, and many programs are lead by faculty. This kind of volunteerism, however, cannot replace the focus and effectiveness of a full-time professional dedicated to creating and nurturing our educational initiatives. The Executive Director for Operations, Dr. Kevin Ausman, has responsibility for directing the day-to-day center operations and those center-wide programs not specifically focused on education. This includes developing industrial outreach programs, coordinating center-wide research activities (such as the annual conference, seminars, and research workshops), and acting as the contact point for NSF questions and reporting. While much of Dr. Ausman’s efforts in these early months have been focused on start-up issues, in future years he will actively coordinate faculty efforts to identify industrial affiliates for the center and develop center-industry partnerships by working closely with the Rice Office of Technology Transfer.

Also as originally proposed, CBEN administrative support includes a center business manager, Associate Director, Shannon Carpenter, responsible for all center-wide purchasing, accounts, and financial reporting. A staff assistant, cost-shared by the Rice Jones School of Management and located in their building, is responsible for coordinating industrial outreach programs such as the Rice Alliance Forums, the entrepreneur workshops, and the annual center conference. A receptionist/secretary provides a daily presence in our offices, fielding phone calls and information requests. Part-time undergraduate help during the school year is also available for specific project development.

In addition to this center staff, CBEN supports with significant Rice cost-sharing two PhD level technical positions for managing shared instrumentation. The first position, hired in February of this year, Dr. Sean Moran, is responsible for maintenance and training in bioanalytical instrumentation, primarily NMR. We are currently searching for the second shared instrumentation position, which will be specialized in electron and force microscopies. These positions contribute to the development of a shared instrumentation infrastructure on the Rice campus, and will participate in graduate student education through training and workshops.
10. Publications

10.1 Publications

10.1.1 Primary CBEN Support

10.1.2 Partial CBEN Support


10.1.3 Use of Shared Facilities


10.2 Disclosures, Patents

10.2.1 Disclosures


10.2.2 U.S. Patent Applications

11. Biographical Information
The following pages contain biographical information for these new center faculty:

- Cecilia Clementi
- Rebekah Drezek
- Jason Hafner
- Jeffrey Hartgerink
- Doug Natelson
- Bruce Weisman
- Michael Wong
Dr. Cecilia Clementi
CURRICULUM VITÆ AND STUDIORUM

Dr. Cecilia Clementi
Rice University
Department of Chemistry MS-60
6100 Main street
Houston, Texas, 77005-1892, USA

Telephone: (713)-348-3485
Fax : (713)-348-5155
e-mail: cecilia@rice.edu
URL: http://leonardo.rice.edu/~cecilia

Education and Qualifications:

10/2001–present : Assistant Professor at Rice University, Department of Chemistry
10/1998 : Ph.D. degree in Physics, full marks cum laude,
International School for Advanced Studies (SISSA/ISAS), Trieste (Italy).
10/1996 : M.Sc. degree in Physics, full marks cum laude,
International School for Advanced Studies (SISSA/ISAS), Trieste (Italy).
3/1995 : Laurea (B.Sc.) degree in Physics, full marks (110/110) cum laude,
University of Florence, Firenze (Italy).
1985–1990 : Scientific Liceum, Firenze (Italy), graduated with full marks (60/60).

Awards:

- Norman Hackerman - Welch Young Investigator award, 2001–2003
- La Jolla Interfaces in Science (LJIS) fellowship (supported by the Burroughs Wellcome Fund), 1999–2001.
- Prize to the best contributed paper, at the XV General Conference of the Condensed Matter Division of the European Physical Society, Baveno-Stresa (Italy), 22-25 April 1996.

Selected publications:

- “Prediction of folding mechanism for circular-permutated proteins”
- “How native state topology affects the folding of Dihydrofolate Reductase and Interleukin-1β”,
- “Topological and energetic factors: what determines the structural details of the transition state ensemble and “on-route” intermediates for protein folding? An investigation for small globular proteins”,
- “Folding Lennard-Jones proteins by a contact potential”,
- “Protein design is a key factor for subunit-subunit association”,
- “Determination of interaction potentials of amino acids from native protein structures: Tests on simple lattice models”,
- “Folding, design and determination of interaction potentials using off-lattice dynamics of model heteropolymers”,
ASSISTANT PROFESSOR REBEKAH A. DREZK


RECENT POSITIONS: Assistant Professor of Bioengineering, Rice University (2002-); Visiting Research Associate, Bioengineering, Rice University (2001); Odyssey Fellow, M.D. Anderson Cancer Center (2001)

RESEARCH INTERESTS: biophotonics, biological applications of optical spectroscopy and imaging, computational electromagnetics, light scattering, signal and image processing


RELEVANT PUBLICATIONS (from over 15 publications, 25 abstracts, and 4 U.S. Patent Applications)

Jason H. Hafner

Physics & Astronomy, MS-61
Rice University
PO Box 1892
Houston, TX 77251-1892

Education and Professional Positions

**Assistant Professor** (2001 - present)
Department of Physics and Astronomy
Rice University

**NIH Postdoctoral Fellow** (1998 - 2001)
Department of Chemistry and Chemical Biology
Harvard University
Advisor: Prof. Charles M. Lieber

Department of Physics and Astronomy
Rice University
Advisor: Prof. Richard E. Smalley

**B.S. in Physics** (1989-1993)
Department of Physics
Trinity University

Awards

- National Institutes of Health Postdoctoral Fellowship, 1999-2001
- Welch Foundation Predoctoral Fellowship, 1994-1998
- Rice Fellowship, 1993-1994
- Presidential Scholarship (Trinity University), 1989-1991

Recent Presentations


Selected Publications


Jeffrey D. Hartgerink, Ph. D.

Department of Chemistry
Northwestern University
2145 Sheridan Rd.
Evanston, IL 60208  
(847) 491-5952 office
Northwestern University (847) 491-3010 fax
j-hartgerink@northwestern.edu
http://pubweb.nwu.edu/~jha463

PROFESSIONAL EXPERIENCE AND EDUCATION

Assistant Professor, Department of Chemistry
Rice University • Houston, TX (starting July 1st, 2002)

Postdoctoral Fellow, Advisor: Samuel I. Stupp
Northwestern University • Evanston, IL (1999 - 2002)

Ph.D. in Macromolecular and Cellular Structure and Chemistry
The Scripps Research Institute • La Jolla, CA (1993-1999)

A.B. in Chemistry and Biology, magna cum laude
Washington University • St. Louis, MO (1989-1993)

SELECTED PUBLICATIONS


SELECTED PRESENTATIONS


*Osaka University Macromolecular Symposium*, Osaka, Japan, June 1995, talk entitled, “Peptide-Based Nanotubes (A New Class of Functional Biomaterials)”.

Vitae—Douglas Natelson, Assistant Professor in Physics and Astronomy, Electrical and Computer Engineering

Mailing Address: Rice University, Department of Physics and Astronomy MS 61, P. O. Box 1892, Houston, Texas 77251-1892. Telephone: (713) 348-3214 e-mail: natelson@rice.edu

Professional Preparation

Princeton University Engineering-Physics (MAE) BSE summa cum laude 1993
Stanford University Physics Ph. D., 1998

Appointments

2000–present Assistant Professor, Dept. of Physics and Astronomy, Rice University.
2001–present Assistant Professor, Dept. of Electrical and Computer Engineering, Rice University.

Selected publications


Collaborators & Other Affiliations

Collaborators: Dr. R.L. Willett, Dr. L.N. Pfeiffer, Bell Laboratories; Prof. Julia Hsu, University of Virginia; Dr. R.B. van Dover, Agere Systems; Dr. Paul Clem, Sandia National Laboratory.
Graduate and Postdoctoral Advisors: Graduate Advisor—Prof. D.D. Osheroff, Department of Physics, Stanford University; Postdoctoral Sponsor—Dr. R.L. Willett, Bell Laboratories, Lucent Technologies.
Thesis Advisor and Postgraduate-Scholar Sponsor: L. Yu, B. Hamadani, S. Lee, A. Trionfi, graduate students (current)
Curriculum Vitae – Robert Bruce Weisman

Address
Department of Chemistry, MS-60
Rice University
P.O. Box 1892
Houston, Texas 77251
Telephone: 713-348-3709    e-mail: weisman@rice.edu

Positions Held
1993 - Professor of Chemistry, Rice University
1984 - 1993 Associate Professor of Chemistry, Rice University
1979 - 1984 Assistant Professor of Chemistry, Rice University
1977 - 1979 Postdoctoral Fellow, University of Pennsylvania

Education
Ph.D. in Chemistry       University of Chicago, March 1977
B.A. in Chemistry        Johns Hopkins University, May 1971

Honors
Alfred P. Sloan Research Fellow 1985 - 1989
National Science Foundation Postdoctoral Fellow 1977 - 1978
Fannie and John Hertz Foundation Fellow 1973 - 1976
University of Chicago Departmental Fellow 1971 - 1972
National Science Foundation Predoctoral Fellow 1971 - 1973
Phi Beta Kappa 1970

Professional Service
Member-at-Large, Fullerenes Group of The Electrochemical Society 2000 - 2002
Fullerenes Symposium Session Organizer, National Meetings of The Electrochemical Society 2000 - 2002

Scientific Society Memberships
American Association for the Advancement of Science
American Chemical Society
American Physical Society
The Electrochemical Society
Sigma Xi

Research Areas
Photophysics and photochemistry
Fullerenes and carbon nanotubes
MICHAEL S. WONG

Rice University
Department of Chemical Engineering, MS-362
Houston, TX 77251-1892

Phone: 713-348-3511
FAX: 713-348-5478
mswong@rice.edu

EDUCATION

<table>
<thead>
<tr>
<th>Institution</th>
<th>Program</th>
<th>Degree</th>
<th>Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>California Institute of Technology</td>
<td>Chemical Engineering</td>
<td>B.S.</td>
<td>1994</td>
</tr>
<tr>
<td>Massachusetts Institute of Technology</td>
<td>Chemical Engineering Practice</td>
<td>M.S.</td>
<td>1997</td>
</tr>
<tr>
<td>Massachusetts Institute of Technology</td>
<td>Chemical Engineering</td>
<td>Ph.D.</td>
<td>2000</td>
</tr>
<tr>
<td>University of California, Santa Barbara</td>
<td>Chemistry and Biochemistry</td>
<td></td>
<td>2000</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2001</td>
</tr>
</tbody>
</table>

EXPERIENCE

Assistant Professor of Chemical Engineering (2001 – present)
Rice University, Department of Chemical Engineering
Nanostructure engineering of materials; heterogeneous catalysis; reaction engineering;
surface chemistry; green chemistry; porous molecular sieve materials for bioseparations

Postdoctoral Research (2000 – 2001)
UCSB, Department of Chemistry and Biochemistry
Organic-inorganic composite materials synthesis and characterization via integration of
biofunctionality at multiple length scales; quantum dots; polypeptide chemistry

Department of Chemical Engineering, MIT
Thesis title: Supramolecular Templating of Mesoporous Zirconia-Based Nanocomposite
Catalysts
Solid acid catalysis with an emphasis on materials synthesis via nanostructure processing;
supramolecular templating; hydrothermal synthesis
Minor: Material Science and Engineering

PROFESSIONAL SERVICES

American Institute of Chemical Engineers Annual Meeting Symposia Organizer (2000, 2001)
American Chemical Society, Materials Research Society, Sigma Xi Member
ACS, Elsevier Journals, Referee (2001)
Rice University, Shared Equipment Authority, Advisory Board (2001)
Rice University, Environmental and Energy Systems Institute, Advisory Board (2001)
Rice University, Will Rice College, Faculty Associate (2001)
MIT Institute Committee on Undergraduate Admissions and Financial Aid (1997, 1998)
MIT Institute Committee on Copyrights and Patents (1997, 1998)

PAST ADVISORS

Jackie Y. Ying, MIT, graduate advisor
Galen D. Stucky, UCSB, postdoctoral advisor
12. Honors and Awards

Andrew R. Barron
2002 Norman Hackerman Award in Chemical Research for contributions to expanding knowledge of inorganic chemistry, presented by the Welch Foundation.

Rebekah Drezek
Invited speaker, IEEE International Conference on Biomedical Imaging.

Alberto Montesi
University of Bologna (Italy) alumni scholarship.

Matteo Pasquali
NSF CAREER award.

Richard Smalley
25 Year Service Award presented by Rice University.
13. Nuggets

**13.1 Break a leg with new bone replacement nanocomposites**
Healing a broken bone isn’t always as easy as wearing a cast. For millions of Americans, new bone growth needs the encouragement of temporary artificial scaffolds which encourage the body to heal itself. At Rice University, Tony Mikos and Andy Barron teamed forces to fill the caps between broken bones with injectable bone replacement polymers filled with nanoscopic alumina. Like pebbles in cement, the alumina nanoparticles strengthen the polymer matrix allowing it to support more weight during the healing process. It wouldn’t have worked without nanotechnology, though: particles larger than 50 nanometers would scatter the visible light used to harden the polymer.

**13.2 A different kind of sponge: nanoparticles soak up cadmium**
Researchers at Rice University have found a new way to treat toxic waste: let nanoparticles do the trick. The amount of available cadmium in water samples was reduced significantly when titania nanoparticles were introduced. Dr. Mason Tomson speculates that the minute crystallites have surfaces which bind strongly to cadmium ions. Like a mobile ion scavenger, the nanocrystals diffuse throughout the solution soaking cadmium onto their surfaces until they are full. The smaller the crystallites, the more surface they have available for sorption. Its estimated that in a teaspoonful of nanocrystals, there is as much available surface as a trampoline, which could clean up even highly concentrated cadmium waste.

**13.3 Twisted room-temperature ice**
Water in a drinking-straw is a liquid. But shrink that straw down to fifty-million times smaller, and that same water turns to ice, even at everyday temperatures. This remarkable discovery by Rice University researchers Jianpeng Ma and Richard Smalley was made using computer simulations of water inside tiny, hollow carbon nanotubes. This particular form of ice has the water molecules lined up in twisting rows down the center of the tubes. Dr. Smalley proposes that this is the perfect arrangement for the system to conduct protons, a synthetic way to achieve a goal central to the functioning of healthy biological cell membranes.