

Summary of IGERT Research Theme

The research theme for this IGERT, the study of materials whose properties are dominated by their nanoscale structure, unifies the chemistry, physics, and engineering of materials with three primary thrusts:

1) **Synthesis and Properties of Nanolaminates and Functionally Graded Materials. (Belitz, Cohen, Haydock, DC Johnson, Keszler, Kevan, Linke, Tate, and Wager).**

The electrical, magnetic, thermal, and optical properties of nanolaminated and functionally graded materials depend on the design details of their nanostructure. Understanding and controlling this requires developing synthetic techniques, optimizing processing parameters to minimize defect densities, measuring the change of properties as a function of nanostructure, analyzing how these materials function in devices, and developing theoretical frameworks to account for observed structure-property relationships. All of these tasks provide numerous opportunities for developing new and useful types materials including thermoelectrics, thin-film photovoltaics, giant magnetoresistance materials, transparent electronics, optical and electrooptical devices, as well as technological applications of superconductivity. Researchers in this group will address three key areas that critically limit the development of nanostructured materials for application in these technologies: • develop *scalable* synthetic approaches to nanolaminates and functionally graded materials; validate these approaches via device demonstrations

- develop techniques both to characterize the defect properties and reduce such defect densities to levels where properties are dominated by the nanostructure, facilitating the realization of practical nanoengineered devices
- develop and understand the structure-function relationships between the nanostructure in these materials and their resultant physical properties

2) **Production, Assembly and Investigation of Nanoparticle-based Materials: Toward Functional Nanoparticle Materials and Devices. (Chang, Deutsch, Gregory, Guillemin, Hutchison, E Johnson, Lonergan, Paul, Reed, Remcho, Taylor, and Wang).**

Researchers in this group are unified in the common goals of synthesizing/manufacturing welldefined, highly functionalized NPs; organizing arrays of NPs; understanding the properties of individual NPs, NP arrays and hybrid nano/mesoscale materials; and realizing functional NPbased devices. In the synthesis of NPs, new materials are being prepared with highly refined properties for electronic and optical applications. In addition, microchannel reactor approaches are being explored for high volume, environmentally benign synthesis of these nanomaterials. In the assembly of NP arrays, molecular templates and functionalized surfaces are being used to fabricate assemblies of NPs not accessible with traditional lithography or to interface nanostructures with mesoscale structures. Optical and electronic investigation of individual nanostructures and arrays will provide a fundamental understanding of their properties and provide a foundation for their use in sensors, quantum logic gates, photonics, and photovoltaics. Interdisciplinary aspects of this thrust group combine biological, chemical, physical and engineering approaches to new materials, the fundamental understanding and applications of complex material systems, and the manufacture of matter with nanoscale spatial organization.

3) Molecularly Programmed Dynamic Assemblies (Branchaud, Haley, Hutchison, DW Johnson, Linke, Liu, Parthasarathy, Rochefort, Tyler).

The object of this thrust group is to create artificial molecular machines and functional materials with specific functional and dynamic properties. The group takes a cradle-to-grave approach, with the vision to actually program in the eventual degradation of the molecular assemblies. The group aims (i) to create synthetic molecular machines capable of performing mechanical tasks, (ii) to equip these machines with sensing capability, and (iii) to program the assemblies to autodegrade after a certain time or when exposed to a specific chemical environment. Molecules and molecular assemblies will be rationally designed with the objective of constructing single and multiple motors that can be integrated with nano- and microstructures, and whose physical performance can be measured. Molecular dynamics and Brownian dynamics modeling are an integral part of this effort. To incorporate sensors into molecular motor systems, the group develops new recognition motifs for a variety of metal ions and small organic molecules, it investigates the dynamic photophysical properties of the new recognition agents and their hostguest and/or metal-ligand complexes; and it studies the dynamic self-assembly of these supramolecular structures. Finally, the team aims to identify the relevant reaction and environmental parameters that affect and determine the degradation of molecular assemblies and functional materials. The specific goal is to identify those factors that control the onset of degradation and the rate of degradation so that adjustment of these parameters will lead to programmed degradation. A dual approach of experiment and modeling is being used to attack the problem of the molecular interpretation of degradation and to correlate assembly morphology with degradation properties.