

Senior Scientist Mentor Program

<u>Institution</u>	<u>Awardee</u>	<u>Department</u>	<u>Area of Interest</u>
2010			
California Institute of Technology	John D. Roberts	Chemistry and Chemical Engineering	We progress in our search for understanding the principles of what influences the preferences for the gauche and trans conformers, usually in compounds of the type X-CH ₂ -CH ₂ -Y, where X and Y can be the same or different groups, we are now searching for general principles governing three easily recognized contributors to preferences; 1. intramolecular hydrogen bonds, 2. electrostatic interactions by charged atoms in X and Y and 3. steric hindrance.
Cornell University	George Hess	Molecular Biology & Genetics	We recently developed rapid reaction techniques suitable for investigating membrane-bound proteins, neurotransmitter receptors, with a microsecond-millisecond time resolution. Supported undergraduates will use the techniques to investigate the mechanisms of reactions mediated by wild-type and mutated GABA(A) receptors in single cells, and identify small organic molecules that potentiate the function of the mutated receptor. The mutations have been linked to epilepsy. The students will learn chemical approaches to interesting biological problems in an interdisciplinary project.
Lafayette College	Joseph Sherma	Chemistry	Thin layer chromatography will be used to determine differences in amounts of various compound classes in the feces and urine of mice experimentally infected with the blood fluke <i>Schistosoma mansoni</i> . This method, which is adaptable for use with humans, is simpler and faster than fecal examination presently used to detect schistosome eggs in host stool. Analysis of infected mouse organs will be performed to obtain a more complete understanding of the infection induced metabolic changes.
Michigan State University	James Dye	Chemistry	Alkali metals in the pores of silica gel are convenient and powerful reducing agents that were developed by us and are now commercially available. Undergraduates will study the nature of these materials as a function of temperature and composition as they range from nanoscale metal crystallites in the pores to metal cations and electrons, to materials with Si-Si bonds.

Senior Scientist Mentor Program

<u>Institution</u>	<u>Awardee</u>	<u>Department</u>	<u>Area of Interest</u>
New York University	David Schuster	Chemistry	The Schuster group at NYU has been involved in the design and synthesis of porphyrin-fullerene hybrid structures with different types of linkers with the aim of studying how the rates of photoinduced electron transfer and subsequent charge recombination depend on molecular architecture. Recently, we have concentrated on materials in which chromophores are mechanically linked, as in rotaxane and catenane architectures. Synthesis of such novel structures in high yields has been possible by employing metal-templating methodology along with "click" cycloaddition chemistry to close rings and extend chains. The studies described in this proposal represent further development of this experimental foray into fullerene-based topologically diverse nanoscale photosynthetic model systems possessing long-lived charge separated states, building on recent studies with strong undergraduate participation.
Oberlin College	Norman Craig	Chemistry and Biochemistry	A combined spectroscopic-quantum chemical method determines equilibrium structures accurate to 0.001 Å for small molecules. Rotational constants for the ground state are obtained from the analysis of pure rotational microwave spectra or from vibration-rotation transitions in high-resolution infrared spectra. A full set of isotopic modifications are synthesized and studied. The high accuracy of these structures reveals structural consequences of electronic effects. Pi-electron delocalization in butadiene is evident in lengthened "double" bonds and a shortened "single" bond. A preliminary structure for the C6 backbone of cis-hexatriene shows greater structural effects of pi-electron delocalization. Current studies include cis- and trans-hexatriene and the impact of fluorine substitution on the isomers of 1,4-difluorobutadiene.
Oregon State University	Joseph Nibler	Chemistry	This project will allow student participation in the synthesis and spectroscopic analysis of propellane, bicyclopentane, and spiropentane, organic molecules with high ring strain and interesting bonding. Students will obtain laboratory experience with vibrational-rotational spectroscopy at state-of-the-art resolution (0.0015 cm ⁻¹) and with the analysis of the complex spectral patterns to obtain accurate molecular parameters. The results will serve as useful new tests of theoretical predictions from ab initio quantum calculations at the anharmonic level.
Purdue University	Ronald Andres	School of Chemical Engineering	The aim of this project is to synthesize bimetallic nanoparticles using a unique aerosol reactor developed in the Purdue laboratory of Professor Andres and to study the applicability of these particles as catalysts for the water-gas shift reaction and as nanoparticle agents for non-invasive detection and treatment of cancer.

Senior Scientist Mentor Program

<u>Institution</u>	<u>Awardee</u>	<u>Department</u>	<u>Area of Interest</u>
The Pennsylvania State University	Ronald Danner	Chemical Engineering	The removal of the last traces of monomers and solvents from polymers is especially important for safety and health reasons. The inverse gas chromatography technique will be used to measure the solubility and diffusivity of solvents in polymers at low solvent concentrations. Data will be obtained and models evaluated for the most prevalent hazardous materials in poly(vinyl chloride) - phthalates and dibenzofuran. This will expose the student to technical as well as social issues.
University of California, Los Angeles	Charles Knobler	Chemistry and Biochemistry	In viruses the genome is surrounded by a container that often consists of multiple copies of a single protein. Some viral RNAs and proteins self-assemble in solution to form infectious viruses. The protein can by itself assemble into a variety of structures, depending on pH and ionic strength. We have argued that the polymorphism depends on protein charge; we propose to test this by examining self-assembly of mutant proteins in which the charge is varied.
University of Illinois at Chicago	Cynthia Jameson	Chemical Engineering	We prepare porous alumina by anodization of Al metal in the form of a hollow cylinder. The highly ordered porous alumina with tunable pore size serves as the support to form pore-spanning lipid bilayers attached electrostatically to the functionalized rims of the nanoporous surface, thus creating an artificial membrane with dimensions of the order of square centimeters. Incorporating this into a toroid cavity detector permits NMR spectroscopy and imaging of molecules along the transport path.
Wake Forest University	Ronald Nofle	Chemistry	New thiophene monomers, both linear and fused-ring, will be synthesized and oligomerized to form low band-gap materials for potential use in solar devices and organic light-emitting diodes. These thiophene monomers will also be functionalized with carboxyl groups suiting them for use as linkers (ligands) in metal-organic framework materials having a range of cavity sizes depending upon the structure of the linker. These materials have potential use as selective solvent adsorbants.