2012-2013 OSU MATERIALS RESEARCH SEED GRANT PROGRAM AWARDS

The **OSU Materials Research Seed Grant Program** provides internal research funding opportunities through three distinct Funding Tiers designed to achieve the greatest impact for seeding and advancing excellence in materials research of varying scopes. The OSU Materials Research Seed Grant Program is jointly funded and managed by the Center for Emergent Materials (CEM), the Center for Electronic and Magnetic Nanoscale Composite Multifunctional Materials (ENCOMM), and the Institute for Materials Research (IMR).

We are excited to announce that after a thorough internal and external review process, nine awards have been made to fund innovative and exciting materials research on campus through the OSU Materials Research Seed Grant Program. These awards total $540,000 in internal research funding to 24 OSU researchers in eight departments.

2012-2013 Proto-IRG Grants

Proto-IRG Grants provide funds up to $100,000/year per award in direct costs, require one Principal Investigator (PI) and two Co-Principal Investigators (Co-PIs), and may have unfunded collaborators. Proto-IRG Grants are awarded with the goal of developing new Interdisciplinary Research Groups (IRGs) that could be incorporated into the renewal proposal that will be submitted by the CEM to the NSF MRSEC program in 2013. Three Proto-IRG Grants were awarded this year:

Band Structure Engineering of Si/Ge/Sn Graphane Analogues

Principal Investigator: Joshua Goldberger, Chemistry; Co-Investigators: Wolfgang Windl, Materials Science and Engineering; Jay Gupta, Physics

Abstract: Graphene's success has shown that it is not only possible to create stable, single atom thick sheets of a layered material, but that these materials can have fundamentally different electronic structures than their parent that are significantly influenced by the environment. We seek to build a competitive, multidisciplinary IRG team comprised of chemists, physicists, and engineers devoted to developing unique single-layer 2D materials, understanding how their properties can be manipulated through surface and atomic substitutions, and building prototype devices that exploit their material advantages. Our

experimental focus will be the creation of silicon, germanium, and tin graphane analogues, or *"silicanes," "germananes*," and *"stannananes,"* since, contrary to graphene, these systems can be chemically functionalized without disrupting their electronic state. Modeling predicts that functionalization can produce systems with either direct or indirect, tunable band gaps ranging from 1.4-2.9 eV for Ge and Si. We will compare the relative influence of surface functionalization and substitutional doping on electronic behavior of single-layer thick materials via modeling, scanning tunneling microscopy, and transport measurements. This dramatic tailoring of the band structure with surface functionalization is truly only possible on these single atom-thick materials, and can offer unprecedented control towards the rational design of optoelectronics, thermoelectrics, spintronics, and chemical/biochemical sensors.

Thermal Spintronics: Materials for Enhanced Heat-Spin Interactions

Principal Investigator: Roberto Myers, Materials Science & Engineering; Co-Investigator: Joseph Heremans, Mechanical & Aerospace Engineering; Collaborators: Ezekiel Johnston-Halperin, Physics; David Stroud, Physics

Abstract: Thermal spintronics combines phenomena in spin-physics and thermoelectronics. Our team has contributed to this field in the last two years by: measuring the spin-Seebeck effect in ferromagnetic semiconductors, the phonon-drag enhancement of spin-Seebeck, and observation of spin-Seebeck in nonmagnetic materials. Spin-thermopower is now three orders of magnitude larger than the original measurements, and on par with charge-heat thermopower. We now focus on a class of materials to study thermo-spin phenomena in order to enhance their magnitudes: strongly bonded materials (AlN, diamond) for enhanced phonon-drag, and narrow gap/zero gap materials (InSb, Bi) for enhanced spin-orbit coupling.

Functional Dynamics of DNA Scaffolded Materials

Principal Investigator: Michael Poirier, Physics; Co-Investigators: Chris Hammel, Physics; Christopher Jaroniec, Chemistry; Carlos Castro, Mechanical and Aerospace Engineering; Collaborator: Ezekiel Johnston-Halperin, Physics

Abstract: The physical and material principles required to design and prepare functional nanometer scale devices is largely unexplored. This Proto-IRG proposal aims to investigate evolved and engineered materials that use DNA as the underlying structural unit. We will create DNA scaffolded nanostructures assembled by DNA origami that are integrated with proteins. This will allow us to construct complex 3D structures that incorporate structural dynamics into their function. We will first investigate the dynamics of these structures with single

molecule fluorescence and force measurements. We will also continue to develop single molecule electron paramagnetic resonance (smEPR) measurements to investigate nanostructural dynamics. smEPR will enable us to measure a wide range of time scales (nanoseconds to seconds) on a single nanostructure. By combining tools from engineering, biology, chemistry and physics, we seek to understand the dynamics of organic nanometer size materials that connect the underlying structure to a functional output.

2012-2013 Multidisciplinary Team Building Grants

Multidisciplinary Team Building Grants provide funds up to $60,000/year per award in direct costs, require one PI and one Co-PI, and may have unfunded collaborators. The goal of the Multidisciplinary Team Building Grants is to form multidisciplinary materials research teams that can compete effectively for federal block-funding opportunities. Two Multidisciplinary Team Building Grants were awarded this year:

Using Neutron Depth Profiling for the Characterization of Current Collectors in Lithium Ion Batteries

Principal Investigator: Marcello Canova, Mechanical and Aerospace Engineering;
Co-Investigator: Raymond Cao, Mechanical and Aerospace Engineering;
Collaborator: Anne Co, Chemistry

Abstract: Lithium-ion (Li-ion) batteries are a key technology for the electrification of automobile. However, a lingering concern is the reliability and cycle life of the cells when subjected to diverse usage factors. Despite the research efforts in understanding the degradation of Li-ion cells and how to mitigate their effects, there is still a gap in the ability to transfer the knowledge on the analysis of degradation in cathode and anode materials to the development of system-level models that can support cell manufacturers and system integrators. The objective of this project is to launch a multi-disciplinary research team combining expertise in nuclear analytical methods, material characterization, analytical electrochemistry, modeling and model-order reduction to bridge the fundamental physicochemical studies with the system-level optimization and control. This innovative approach to research will be effective not only in improving the fundamental understanding of aging, but also in investigating new cathode and anode materials for the next generations of Li-ion batteries. As a case study, the degradation due to intercalation of Lithium in the current collectors will be investigated. This requires understanding the underlying physical and chemical processes, quantifying their impact on the electrical performance of current collectors, and finally relating to the system-level battery aging.

Engineered Heart Tissue: A Multidisciplinary Team Centered on Scaffold Structure and Mechanics

Principal Investigator: Jianjun Guan, Materials Science & Engineering; Co-Investigators: Gunjan Agarwal, Biomedical Engineering; Peter Anderson, Materials Science & Engineering

Abstract: A multidisciplinary team spanning three academic departments is proposed to enhance both the intellectual merit and broader impacts of engineered heart tissue research at The Ohio State University. The intellectual merit is to understand how the material design of 3D fiber scaffolds, coupled with cells that can secrete collagen with tunable properties, can be used to direct stem cell differentiation into heart cells. A structured set of key aims will demonstrate the ability of 3D fiber arrays to regulate differentiation, and then correlate this differentiation with the material properties of the collagen matrix and the material design of the fiber scaffold. This effort draws on recent developments of how 2D material environments affect cell differentiation, by expanding to 3D fibrous structures that are inherent in heart tissue. The broader impacts are to support two graduate students in a unique educational setting not available in a single academic setting. It will identify and strengthen a multidisciplinary team for future block grant funding not currently available to OSU researchers, and foster new interaction between the medical and physical sciences at OSU.

2012-2013 Exploratory Materials Research Grants

Exploratory Materials Research Grants provide funds up to $40,000/year per award in direct costs, require one PI, and may have Co-PIs and/or unfunded collaborators. The goal of the Exploratory Materials Research Grants is to enable nascent materials research to emerge to the point of being competitive for external funding. Four Exploratory Materials Research Grants were awarded this year:

DNA-based Molecular Actuators for Novel Smart Material Systems

Principal Investigator: Carlos Castro, Mechanical and Aerospace Engineering; Co-Investigators: Marcelo Dapino, Mechanical and Aerospace Engineering; Haijun Su, Mechanical and Aerospace Engineering

Abstract: The objective of this research is to develop DNA-based smart molecular actuators (SMA) using the recently developed structural nanotechnology scaffolded DNA origami for application in novel smart material systems. These SMA will be capable of translating nanoscale actuation via molecular interactions to programmed collective motion at the micron scale. Within the scope of this work, we will design and fabricate DNA origami structures capable of structural shape changes using DNA strand displacement techniques. Structures will be joined

together in a hierarchical assembly following a kinematic design approach so that shape changes at the individual structure level yield programmable micron-scale collective motion. The long-term goal of this work is to develop materials capable of coupling nanoscale actuation via molecular interactions to motion of macro-scale engineering materials including traditional smart materials (i.e. piezoelectric or shape memory polymers). This seed grant will help us lay the groundwork for future proposals to seek funding for the development of novel biologically active smart materials.

New Approach to Electromagnetic Interference (EMI) Shielding of Plastic Parts: Nanopaper In-Mold Coating

Principal Investigator: Jose Castro, Integrated Systems Engineering; Co-Investigator: L. James Lee, Chemical and Biomolecular Engineering

Abstract: There are many applications where light weight materials that provide EMI shielding are required. For example, personal computers, aerospace components, automotive components, military component housings, etc. There are two approaches used to date to achieve EMI shielding for plastic products. One is coating with conductive metals or particles. Another method is to use polymer composites filled with conductive fillers such as carbon nanofibers and carbon nanotubes. We propose to develop a new better approach to provide EMI shielding as well as surface protection for thermoplastics by combining the use of in-mold coatings and Carbon Nanofiber (CNF) nanopaper. We use a layer by layer spray approach to manufacture the nanopaper. Critical to the success of our approach is the surface modification of the CNF. This is important not only in enhancing the mechanical and electrical properties of the nanopaper but also in controlling the dispersion in the suspending fluid. Due to the intrinsic van der Waals attraction, nanoparitcles are usually tightly entangled obtaining a uniform dispersion is challenging thus we need both mechanical and surface modification.

Modifying the Kinetics and Selectivity of CO2 Electroreduction through Ionic Liquid – Electrode Interactions

Principal Investigator: Anne Co, Chemistry and Biochemistry; Collaborators: Aravind Asthagiri, Chemical and Biomolecular Engineering; David Cole, Earth Sciences

Abstract: This proposal seeks to understand the role of solvent and ionic interactions on stabilizing surface species in the CO2 electroreduction pathway. Specifically, we propose to investigate the role of ionic liquids in the electroreduction of CO2. Ionic liquids, especially those having quaternary ammonium centers, have shown great promise in CO2 capture. Our goal is to explore the unique properties of this class of ionic liquids and their interaction with

well-ordered metal surfaces. To accomplish this goal we will apply electrochemical and spectroscopic techniques, and density functional theory calculations on surface species. The scope of this seed proposal is to obtain preliminary data and establish collaborative relationships to pursue future block funding opportunities from NSF, DOE related to CO2 capture, storage and conversion.

Rechargeable Potassium-Air Batteries with High Energy Storage and Efficiency

Principal Investigator: Yiying Wu, Chemistry; Co-Investigator: Sheldon Shore, Chemistry and Biochemistry

Abstract: The objective of this proposal is to create rechargeable potassium (K) - air batteries (KAB). A KAB cell is composed of a potassium metal anode and an oxygen cathode. In comparison with the state-of-the-art Li air batteries, the unique feature of KAB is that the superoxide intermediates from the one-electron reduction of dioxygen molecules can be captured by potassium ions to form potassium superoxide. The use of this *one-electron quasi-reversible* process is expected to increase the reversibility of the oxygen reduction reaction, decrease the voltage gap between discharging and charging, and reduce (or even remove) the use of the electroctalysts in the oxygen electrode. Moreover, a free energy calculation shows the theoretical specific energy is 935 Wh/kg (based on the mass of KO2). This is about 2½ times of the Li-ion battery, and is similar to the zinc-air battery. Furthermore, potassium is the seventh most abundant element. It is appropriate for the large-scale application of batteries. Therefore, KAB should hold great promise for rechargeable batteries with advantages in specific energy, energy efficiency, cycle life and material abundance. With its impact to the battery market, this project is expected to invigorate interdisciplinary collaborations between chemistry, engineering and industry.