THE OHIO STATE UNIVERSITY
IMR Institute For Materials Research
CEM Center for Emergent Materials
encomm Exploration of Novel Complex Materials

2015 OSU MATERIALS RESEARCH SEED GRANT PROGRAM AWARDS

We are pleased to announce that after a thorough internal and external review process, 9 awards have been made to fund innovative and exciting materials research on campus through the 2015 OSU Materials Research Seed Grant Program. These awards total $420,000 in internal research funding to 15 OSU researchers in 5 departments. The program was able to fund 47% of the proposals submitted this year; 9 out of a total 19. Congratulations to the nine research teams whose projects were selected this year for seed grant funding.

2015 Multidisciplinary Team Building Grants

Multidisciplinary Team Building Grants form multidisciplinary materials research teams that can compete effectively for federal block-funding opportunities. Three Multidisciplinary Team Building Grants were awarded this year:

DNA Devices for Probing Nanoscale Physics of Fluids

PI: Carlos Castro, Mechanical and Aerospace Engineering; Co-Investigators: Michael Poirier, Physics; Shaurya Prakash, Mechanical and Aerospace Engineering; Soheil Soghrati, Mechanical and Aerospace Engineering

This research will develop DNA nanodevices to measure fluid properties such as viscosity, shear rate, pressure, and flow velocity at nanometer length scales to enable the study of phenomena such as viscous damping near surfaces, rheology in inhomogeneous solutions, or effects of crowding in polymer solutions, which are currently poorly understood largely due to lack of measurement technology at appropriate length scales. To address this technological gap, we have assembled a team that integrates expertise in design and assembly of DNA nanostructures (Castro), single molecule measurements of structure and dynamics (Poirier), micro- and nano-fluidics (Prakash), and mechanical modeling with an emphasis on structure design and optimization (Soghrati). The goals of this 1-year seed grant are to achieve two key milestones that will provide a strong basis for pursuing external multi-PI funding: 1) demonstrate proof-of-principle measurements of local viscosity and osmotic pressure in unconfined and confined systems, and 2) establish and validate a computational mechanical model that enables design of DNA bundles for specific mechanical properties. If successful, we will be well-positioned to pursue team funding in programs that support studies of complex fluid systems (e.g. polymer solutions, biological systems, hydrogels, etc.), development of sensor technologies, and design of novel material systems.

Studies of Dopant Dynamics Using Microscopy at Atomic Length and Femtosecond Time Scales

PI: Jay Gupta, Physics; Co-Investigator: Enam Chowdhury, Physics

This program is focused on developing an ultrafast scanning tunneling microscopy (UF-STM) technique to study how reduced symmetries influence the dynamics of individual dopants in semiconductors. To overcome the inherently slow instrumental response time, we have designed and built a portable ultrafast oscillator (PUPIL) that can resonantly excite band-to-dopant transitions and is suitable for pump-probe dynamics studies. PUPIL will be integrated with a custom-built low-temperature STM. We will demonstrate UF-STM studies of Er-doped GaAs, whose intra-4 f shell transitions are resonant with the PUPIL wavelength 1.55 μm (200 THz). Er atoms will be deposited *in situ* onto a pristine GaAs (110) surface, cleaved in ultrahigh vacuum. Our UF-STM studies will directly probe how the GaAs:Er dynamics depend on the local environment for the first time. In addition to providing unique insights into an important problem in semiconductor physics, this program will provide a nucleus for future team efforts in physics, chemistry, materials science and electrical engineering.

Skyrmions in Low-Dimensional Chiral Magnets

PI: Mohit Randeria, Physics; Co-Investigators: Roland Kawakami, Physics

This joint experiment-theory project will develop new chiral magnetic materials and gain insights into novel spin textures, called skyrmions, in thin-films. Skyrmion phases exhibit fundamentally new phenomena like emergent electromagnetism and the topological Hall effect, and promise new functionalities for spintronics and memory applications. Our collaboration builds on recent theoretical progress by one of the PIs (*Randeria*) on predicting the enhanced stability of skyrmions exploiting Rashba spin-orbit coupling, together with the experimental expertise of the other PI (*Kawakami*) and our senior collaborator (*Dunsiger*) on molecular beam epitaxy (MBE) growth and characterization of novel magnetic materials. Our proposed research will lay the foundation for a broad-based effort involving the OSU materials community, which will be highly competitive for federal funding.

2015 Exploratory Materials Research Grants

Exploratory Materials Research Grants enable nascent materials research to emerge to the point of being competitive for external funding. Six Exploratory Materials Research Grants were awarded this year:

Investigating Crystallization Mechanisms of Microporous Materials Using Ion Mobility-Mass Spectrometry

PI: Nicholas Brunelli, Chemical and Biomolecular Engineering

This project will seek to determine the intermediate species formed during nucleation and growth of metal-organic frameworks (MOFs) using ion mobility-mass spectrometry (IM-MS). The key challenges for MOFs remain synthesizing novel structures and achieving high yields. These deficiencies originate from a poor understanding of the crystallization mechanism. We hypothesize that we can identify the critical intermediate species responsible for nucleation and growth utilizing ion mobility-mass spectrometry (IM-MS). IM-MS is a two-dimensional separation technique capable of simultaneously providing structure and composition of the molecular-sized species responsible for the final structure and properties of MOFs. This novel application of IM-MS will provide insight not available with other techniques like NMR, XRD, and AFM. The findings will enable discovery of new crystal structures and modification of synthetic conditions to improve crystal phase purity and overall yield. The long term objective of this work is to establish IM-MS as an important characterization method for material crystallization. The system will be expanded to study crystallization of aluminum species for thin film dielectrics, crystallization of aluminum and silicon species for zeolites, and assembly of catalytic intermediates. Important details of these systems are only accessible through the powerful IM-MS system.

First-Principles Study of Dislocation Core Structures and Properties in Multi-Principal-Element Alloys

PI: Maryam Ghazisaeidi, Materials Science and Engineering

Multi-principal-element alloys (MPEAs) are a relatively new class of multicomponent metallic alloys in equal or near equal atomic percent resulting in a high entropy of mixing and unique properties that make them candidate materials for many potential applications. Instead of ordered inter-metallics expected from classic physical metallurgy, simple phases like BCC and FCC have been observed in many MPEA systems. The complex compositions of these alloys lead to interesting phenomena concerning thermodynamics, kinetics, structure and properties where the fundamentals are still open questions. The goal of this proposal is to understand the basic mechanisms affecting the *mechanical* properties of MPEAs. At this point it is not clear whether the deformation mechanisms in MPEAs (e.g. dislocation structures, stacking faults and solute strengthening) are simple extensions from those of conventional alloys. The proposed research will focus on developing new computational tools to investigate dislocation core structures in MPEAs with first principles calculations. The new tools - built from established tools - will enable accurate determination of dislocation core geometries and bonding environments in multi component alloys. The outcome will serve as a building block for a bigger plan to understand the fundamentals of deformation mechanisms in MPEAs.

Direct Imaging of Atomic Scale Electromagnetic Fields in Functional Materials

PI: Jinwoo Hwang, Materials Science and Engineering

We propose to advance differential phase contrast (DPC) imaging in scanning transmission electron microscopy (STEM) to determine the atomic scale electromagnetic fields in functional materials that directly connect to their emergent properties. The new technique will capture the subtle perturbation in the electron probe generated by the fields around individual atoms using a segmented reciprocal-space STEM detector in *in-situ* or *in-operando* conditions, such as under electrical bias. We will establish a fundamental understanding of the exact DPC mechanism at the atomic scale, and the experimental framework for DPC imaging in an aberration-corrected STEM environment. Using the new technique, we will identify the atomic scale electromagnetic structure near defects or interfaces that determines the important properties of complex oxide heterostructures, 2D layered materials and interfaces, and spintronic systems.

Developing Electrodes for Hydrogen Production Based on Robust Biological Catalysts

PI: Hannah Shafaat, Chemistry and Biochemistry

This proposal describes the development and optimization of bioderived and biocompatible devices for electrocatalytic hydrogen production based on simple, robust nickel-substituted rubredoxin (NiRd) proteins immobilized on carbon-based electrodes. Our lab has previously demonstrated high electrocatalytic hydrogen production activity from a mesophilic NiRd protein adsorbed to a graphite electrode. The proposed work will 1) create catalytically active NiRds using proteins derived from a hyperthermophilic organism; 2) develop methods for selective covalent attachment of these catalysts to carbon electrode surfaces; and 3) demonstrate robust catalytic activity under mild aqueous conditions after desiccation, thermal treatment, and prolonged exposure to oxygen. Characterization of these systems in solution and on surfaces will provide insight into the molecular principles governing morphology, surface attachment, and catalytic mechanism; ultimately, these materials can be coupled with light-harvesting moieties for solar fuel production.

Exploration of the Anomalous Hall Effect at Terahertz Frequencies

PI: Rolando Valdés Aguilar, Physics

Although there has been much progress in the last 10 years, both theoretical and experimental, in the understanding of the Anomalous Hall Effect (AHE) and related phenomena such as the Spin Hall Effect (SHE), there has been little to no exploration of these physics at finite frequency, particularly in the terahertz (THz) energy range. Measurements in the frequency domain have the advantage of separating carrier density from transport scattering time effects, and are in the correct energy range of several meV to explore spin-orbit coupling-induced phenomena. The objective of this project is to separate the different transport contributions from the intrinsic AHE that is due to Berry-phase curvature effects by using time domain THz spectroscopy (TDTS). Novel polarization capabilities for TDTS will be utilized to perform high sensitivity THz Hall effect measurements in model systems. These new developments are an achromatic quarter wave plate to generate broadband circular polarization in the THz range, and a highly sensitive polarization modulation technique to detect small Faraday rotation signals at THz frequencies. A variety of systems will be explored, from transition metal ferromagnets to novel double perovskite semimetals.

Development of Epitaxial Film Growth of Group V-VI Topological Insulators by Molecular Beam Epitaxy

PI: Fengyuan Yang, Physics

One of the most exciting frontiers in materials research is topological insulator (TI) heterostructures which exhibit fascinating electronic and spin properties. Supported by CEM and ENCOMM, the PI is building a cluster deposition system in his lab that includes an off-axis sputtering chamber with high-pressure reflective high energy electron diffraction (RHEED) for complex oxide growth and a molecular beam epitaxy (MBE) chamber for TI growth. This Exploratory Materials Research Grants proposal requests funds for supporting a graduate student for one year as well as materials and user fees to develop MBE growth of TI films on various substrates and epitaxial films. We will investigate dynamically driven pure spin transport from $Y_3Fe_5O_{12}$ films into TI films and characterize the inverse spin Hall effect and spin Hall angle in TI films. This experiment will be independently verify the reported extraordinarily large spin Hall angle in TIs. In addition, we will explore interfacial exchange coupling induced ferromagnetism in TI thin films grown on magnetic insulators and search for novel electronics phases such as the quantum anomalous Hall effect in TI films induced by magnetic proximity effect.

About the OSU Materials Research Seed Grant Program

The OSU Materials Research Seed Grant Program provides internal research funding opportunities through two 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 Exploration of Novel Complex Materials (ENCOMM), and the Institute for Materials Research (IMR).