2016 OSU Materials Research Seed Grant Program Awards

We are pleased to announce that after a thorough internal and external review process, 11 awards have been made to fund exceptionally promising, innovative materials research on campus through the 2016 OSU Materials Research Seed Grant Program. These awards total $500,000 in internal research funding to 25 Ohio State researchers from 10 departments in five colleges. The program was able to fund 58% of the proposals submitted this year; 11 out of a total 19. Congratulations to the eleven research teams whose projects were selected this year for seed grant funding.

The 2016 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).

2016 Exploratory Materials Research Grants

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

Direct Structural Determination of Individual DNA Molecules Using Electron Nanodiffraction

PI: Jinwoo Hwang, Materials Science and Engineering; Co-Investigator: Kichoon Lee, Animal Sciences

We propose to develop a new electron nanodiffraction technique in transmission electron microscopy (TEM) that can directly determine the detailed structure of individual DNA molecules. We will use low energy electron nanobeams that can probe the nanoscale sections of individual DNA molecules one by one. The proposed new technique will provide higher resolution and spatial specificity as compared to the current generation cryo-TEM imaging or light-based spectroscopy. The new technique developed through the IMR Seed program will establish the technical foundation to achieve major scientific advances such as the next generation DNA sequencing technology. Here, we will focus on 1) establishing TEM optics and detector geometry to maximize the information limit with low doses, 2) developing a new DNA sample preparation method that ensures high efficiency and minimizes radiation damage, and 3) quantitative data analysis using advanced diffraction simulation algorithms. The expected results of the proposed studies will lead to high impact discoveries that will be published and used for grant proposals to multiple important federal funding opportunities, such as in NIH and NSF.

Molecular Beam Epitaxy Growth of 2D Ferromagnetic Semiconductors

PI: Roberto Myers, Materials Science and Engineering; Co-Investigators: Roland Kawakami, Physics; Wolfgang Windl, Materials Science and Engineering

The 2D transition metal dichalcogenides (TMDs) represent an important and underutilized class of 2D semiconductors because unlike graphene, the TMDs allow for traditional band gap engineering as the composition of (Wx,Mo1-x)(Sy,Se1-y)2 is varied. The recent demonstration of both band gap tuning as well as n-type and-p-type has opened new opportunities for developing 2D semiconductor optoelectronic devices. In particular, Myers and coworkers recently demonstrate p-type MoS2 with Nb doping. Recently, it was predicted that 3d transition metal doped 2D MoS2 should exhibit ferromagnetism. If true, this would represent the first 2D dilute magnetic semiconductors (DMSs). Such a 2D ferromagnetic semiconductor would represent a revolutionary new magnetic system to test fundamental theories on the limits and properties of ferromagnetism in 2D materials. We will synthesis Mn-doped (Mo,W)Se2 using a newly acquired MBE system. If the effort is successful it will open a new field of research in 2D materials with strong implications for applications and basic physics.

An Integrated Experimental-Computational Approach for Determining the Phonon Mean Free Path Spectrum in Semiconductors

PI: Sandip Mazumder, Mechanical and Aerospace Engineering; Co-Investigator: Marat Khafizov, Mechanical and Aerospace Engineering

At the sub-micron scale, the thermal conductivity of a semiconductor material is not a fundamental material property. It is size dependent. This size dependence provides a new and unique “knob” to manipulate its value through nanostructuring. The prerequisite to effectively utilize size effects to tailor the thermal conductivity is to have knowledge of the spectral mean free path of the primary energy carriers in the semiconductor, namely phonons. Data generated by recent pump-probe transient thermo-reflectance (TTR) experimental measurements can be used to directly extract the phonon mean free path spectrum. The challenge, however, is that this requires an intervening advanced model, namely the full seven-dimensional Boltzmann Transport Equation (BTE) for phonons. This project aims to extract the phonon mean free path spectrum directly from TTR measurements by using a parallel solver of the multi-dimensional, transient, frequency-dependent phonon BTE, in conjunction with the Levenberg-Marquardt inverse algorithm. Subsequent to the extraction of the mean free path spectrum, the effective thermal conductivity, and the thermal conductivity accumulation and suppression functions will be determined. Silicon will be used as the candidate material for demonstration of the proposed approach.

Effects of Polymer Adsorption on Dynamics of Model Polymer Nanocomposites for Design of Advanced Tire Tread Compounds

PI: Kurt Koelling, Chemical and Biomolecular Engineering; Co-Investigator: Lisa Hall, Chemical and Biomolecular Engineering

A major challenge in the tire industry is to create materials with good traction (which requires high hysteresis in mechanical strain) that also have low rolling resistance (requiring low hysteresis, but at a somewhat different frequency). Tire tread materials are based on styrene-butadiene rubber potentially containing both silica and carbon black nanoparticles and several other additives, however, to make progress in understanding the physics of how nanoparticles affect polymer behavior, we will investigate simplified materials composed of silica nanoparticles (with and without surface treatment that affects adsorption) and linear, non-crosslinked polymers. We hypothesize that polymer relaxation times, and thus hysteresis, depend significantly on both average polymer-particle interaction strength and on copolymer sequence (where the two types of monomers have different interaction strengths with the particles). Concerted experiments and molecular simulations of the model materials with different monomer sequences will show

how controllable molecular features determine the structure and resulting material properties, and we aim to predict how to adjust the hysteresis at different frequencies. This program will have close ties to industrial research at Cooper Tire and Rubber Company, allowing us to solidify our collaboration in preparation for proposing the work to external funding agencies such as NSF (GOALI program).

Uncertainty Quantification for Model Selection: Evaluating Material Constitutive Models based on Available Data

PI: Stephen Niezgoda, Materials Science and Engineering; Co-Investigator: Oksana Chkrebtii, Statistics

ICME is increasingly being adopted as a strategy to accelerate materials design, discovery, and deployment by replacing expensive experimentation with simulation. This reliance on simulation demands a quantitative assessment of model fidelity and predictive accuracy. The evaluation of materials simulation involves verification and validation (V&V) and uncertainty quantification (UQ). Broadly speaking, V&V is concerned with calibrating model parameters to best reflect the experimental data followed by critically evaluating the model predictions. UQ, on the other hand, involves understanding how error due to incomplete knowledge or uncertainty propagates through the simulation to quantify the expected error in the final property or performance predictions. A complex physics-based material model may not always outperform a simple empirical model, especially when the calibration data is limited. We propose to address V&V and UQ simultaneously as part of a self-consistent Bayesian model selection and inference framework. We will adapt state-of-the-art UQ approaches to track the confidence in model predictions to determine which of the available models is “best" for a given application. A key benefit of this work will be a formal methodology for model selection and a framework for evaluating the adequacy of experimental calibration data, based on the required confidence in model prediction.

Development of a Nanoscale Rheology Sensor in a Microphysiological Model of Tumor Stroma

PI: Jonathan Song, Mechanical and Aerospace Engineering; Co-Investigators: Carlos Castro, Mechanical and Aerospace Engineering; Michael Ostrowski, Cancer Biology and Genetics

It is well established that central to tumor progression are the evolving mechanical and material properties of the extracellular matrix (ECM). It is believed that these changes are conferred primary by the stromal fibroblasts. However, measuring changes in ECM remodeling in tumors that is quantitative and non-invasive in vivo is challenging due to complexities associated with this rapidly evolving tissue. To meet this challenge, we will develop an imaging-based methodology for dynamically measuring fibroblast-generated changes in ECM remodeling and rheology in vitro using micro and nano-scale technology. We will achieve this objective by integrating a nanoscale rheology sensor (NRS) into our microphysiological tumor stroma comprised of fibrillar type I collagen and cancer associated fibroblasts (CAFs) from pancreatic cancer patients. This integrated approach will analyze ECM remodeling with confocal reflectance microscopy and produce dynamic and quantitative stress maps to measure cell-generated changes in ECM rheology. The successful outcome of this research will provide a clearer understanding of the physical mechanisms that promote pro-tumor responses mediated CAFs.

Synthesis and Design of Novel Graphyne and Graphdiyne-Based Metal-Organic Frameworks

PI: Psaras McGrier, Chemistry and Biochemistry

The global demand for new sources of clean energy and the reduction of greenhouse gases have become two of the major focuses in academia and industry. Metal-organic frameworks (MOFs) have emerged as promising materials to help address these issues thanks to their tunable pore sizes and thermal stability

making them useful for gas separations and storage applications. In an effort to find new materials that can continue to aid in these explorations, this proposal focuses on utilizing π-electron conjugated dehydrobenzoannulenes (DBAs) to construct novel two-dimensional (2D) MOFs. DBAs possess triangular pores that can bind small alkali and alkaline earth metals such as lithium and calcium, respectively. Since both metals are known to increase the storage capacity of microporous materials for CO2/H2 on account of electrostatic interactions (CO2) and polarizability (H2) of the atoms, this feature would add a distinct advantage over the current state-of-the-art 2D MOFs. To sum up, this proposal seeks to investigate the following: 1) novel synthetic strategies to construct multipore 2D DBAMOFs that can form metal complexes with lithium and calcium, and 2) how careful selection of lithium or calcium metal-doped ligands can be used to enhance their binding interactions with CO2 and H2.

The Effect of Abutment Material on Wear of Internal Engaging Features of Implants under Cyclic Loading

PI: Fengyuan Zheng, Restorative Sciences and Prosthodontics; Co-Investigators: Damian Lee, Restorative Sciences and Prosthodontics; Jinwoo Hwang, Materials Science and Engineering

The intimate adaptation and engagement between dental implant and abutment, along with clamping force through screw joint, provides retention and resistance and ensures the proper function of an implant supported restoration. A lack of stability can be resulted from wear of engaging components of implant-restoration assembly under cyclic loading and may lead to catastrophic failure, which leads to replacement of the restorative components or implants, which may cause severe morbidity to host site(s). The application of Zirconia, mainly for superior esthetics, as an abutment material has made internal engaging features more susceptible to wear due primarily to greater hardness of zirconia over titanium or titanium alloys. Previous studies have focused on wear pattern of expendable restorative components rather than osseointegrated implant engaging features, which, once damaged by excessive wear, will be more challenging to replace without morbidity of the site. Hence, the purpose of proposed study is to characterize the wear behavior of internal engaging features of a dental implant depends upon the abutment materials (titanium and zirconia), geometrical configuration of the feature, and the nature of loading coupled with different initial torque values. A more rapid wear is expected with Zirconia abutment, lower initial torque, and conventional design. The result of present proposal will contribute in depth understanding of implant-restoration interaction and predictable outcomes of implant supported restorations with different materials. Furthermore, it provides clinic guidance when treatment plan is made and future development of abutment materials.

2016 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:

Ultra Wide Band Gap III-Nitride Semiconductor Materials and Devices

PI: Siddharth Rajan, Electrical and Computer Engineering; Co-Investigators: Jinwoo Hwang, Materials Science and Engineering; Aaron Arehart, Electrical and Computer Engineering

Wide band gap semiconductors such as GaN and SiC are making significant technological impact in areas such as communication, lighting, sensing, and power conversion. Ultra wide bandgap semiconductors with bandgaps exceeding GaN/SiC, such as ultra wide band gap AlGaN alloys, promise even greater device performance and functionality. The objective of the proposed work is to investigate the synthesis, structure, and electronic properties of ultra wide band gap AlGaN-based semiconductors and their heterostructures.

Magnetic Dynamics and Excitations in Skyrmions Stabilized by Thin Films and Multilayers

PI: Chris Hammel, Physics; Co-Investigators: Vidya Bhallamudi and Fengyuan Yang, Physics; David McComb, Materials Science and Engineering

Skyrmions are promising materials for high density, energy-efficient magnetic storage and computing, and present an excellent platform for understanding magnetism where strong spin-orbit coupling plays a major role. We propose to investigate thin film and layered materials that stabilize a robust skyrmion phase over a large range of temperature and magnetic field, and enable nanoscale control of their generation and manipulation using scanned micromagnetic tips. Our team brings together an array of complementary tools that we will use to study of a range of properties: the physical structure (X-ray diffraction and Transmission Electron Microscopy), static magnetic properties (SQUID), magneto-transport (topological Hall effect), magnetic structure (Lorentz Transmission Electron Microscopy and Magnetic Force Microscopy), and magnetic dynamics and excitations (conventional microwave absorption and optically detected magnetic resonance, and magnetic resonance force microscopy). We have grown epitaxial films of FeGe, and our structural, transport and narrow-band resonance measurements indicate the promise of our approach. We request funding for a team to observe and understand skyrmions in epitaxial thin films of B20-phase materials and ultrathin layered materials that enable artificial skyrmions, and to pursue their controlled generation and manipulation using scanned magnetic tips.

Halide Double Perovskites: A New Class of Lead-free Compound Semiconductors

PI: Patrick Woodward, Chemistry and Biochemistry; Co-Investigators: Joseph Heremans, Mechanical and Aerospace Engineering; Roberto Myers and Wolfgang Windl, Materials Science and Engineering

The lead halide perovskites, such as CH3NH3PbI3, possess the electrical and optical properties of conventional semiconductors, but unlike most semiconductors they can be prepared by simple inexpensive methods including deposition from solution. They are suitable for many applications, the most exciting of which is in solar cells where the efficiencies have risen dramatically and are now comparable to single crystal silicon solar cells. Their biggest liability is the toxicity that comes from the presence of lead. The proposed research aims to discover and develop halide double perovskites, a related class of semiconducting materials that potentially possess many of the favorable characteristics of the lead halide perovskites, but without the presence of lead. New materials will be found via computationally guided exploratory synthesis. Routes to growth of single crystals and thin films will be established for promising materials. Detailed characterization of the optical and electrical properties will provide the necessary feedback to design materials with properties that are optimized for use in solar cells, light emitting diodes, scintillators for radiation detection, and p-type transparent conductors.