➢ Understanding real materials of technological relevance (T, Fu)

The research focus in Fu group is to investigate and understand real materials of technological importance by using solid state theory and first-principles density functional calculations. Perspective REU students can choose to participate in any research activity in the following areas, depending on their interests.

(I) Ferroelectric (FE) nanostructures of perovskite oxides: These ferroelectric or piezoelectric perovskites distinguish themselves from other classes of materials, by possessing spontaneous polarization under zero electric field and by being able to efficiently convert electricity into mechanical energy or vice versa. They are widely utilized in energy-conversion devices such as transducers and actuators, robotics, and MEMS[1]. These materials have also been ubiquitously used in ultrasonic imaging for human health, arrays for telecommunications, and military sensors for national security.[2] Furthermore, ferroelectrics often have high dielectric susceptibility, and have been heavily used for energy storages and microelectronics,[2] as well as for nonvolatile random access memories.[3] Our active researches involve the studies of new phase transitions in FE nanoparticles[4], one-dimensional wires[5], symmetry-breaking phase transformation path between two phases of entirely different order parameters[6], vortex switching[7], defect physics in ferroelectrics[8], rigorous definition and computing of LO/TO splitting[9], as well as new morphotropic phase boundary and ultrahigh electromechanical responses[10]. The REU students will use the density-functional theory to calculate the relative phase stabilities of different ferroelectric structures, the magnitudes of atomic off-center displacements, as well as the size of spontaneous polarization using the modern theory of polarization. The REU participants will gain important knowledge on first-principle density functional theory, spontaneous polarization, and ferroelectric physics.

(II) The second area of research is to investigate, understand, and attempt to improve the desirable properties of semiconductor-based organic-inorganic hybrid materials that may yield next generation of solar electric devices (with much improved efficiency) for clean energy, as well as being able to generate new ideas on microelectronics and optoelectronics. Semiconductor-based hybrid materials, synthesized as super-structures with alternating organic and inorganic constituents, combine the advantages of inorganic semiconductors and organic polymers, which are two major types of materials of interest. Purely-organic devices are mechanically flexible, but often suffer low carrier mobility because of weak Van der Waals interaction between molecules. By contrast, inorganic components in *hybrid* materials overcome this limitation and provide many superior features such as high carrier-mobility in thin-film field effect transistors,[11] enhanced electron-hole recombination rate in optoelectronic diodes,[12] and possible doping of spin electrons in magnetic devices[13,14]. The organic components, which serve as the building "glue" to connect the inorganic blocks, provide great flexibility in structure design, and enable the future generation of electronic devices made of hybrid materials to be folded into a very small volume. These hybrid composites can potentially make the dream of "plastic semiconductors" a reality. The research activities in our group include the studies of optical and electronic properties in hybrid single crystal[15,16] $ZnSe(C2H8N2)_{1/2}$, influence of mechanical pressure on the electron properties[17], unusual zero thermal expansion[18], etc. The participating REU students will determine the structure as well as electronic properties of the hybrid materials by using density functional calculations. Students will gain knowledge on the key differences in the physical properties of organic, inorganic, and hybrid solids, and will be exposed to a new field of hybrid materials.

(III) Semiconductors: Semiconductors are the prototypical materials for examining new ideas and theories. New semiconductor technologies prefer to have multi-functional materials that are suitable for multi-purposes and with better performances. For example, seeking the *same* material that can be used simultaneously for high speed electronics,[19,20] sensitive infrared sensors,[21] solid-lighting optoelectronics,[22,23] as well as spin transport in spintronics[24] is of great fundamental and technological relevance. Our research activities include electromechanical response[25] in GaN, crystallographic

orientation dependent electronic properties in InP nanowires[26], polar-to-nonpolar transition[27] in ZnO, giant Rashba spin splitting[28] in BiTeI, δ-doping[29] in SrTiO3, etc. The REU students will calculate the atomic geometry, band structure, optical transition probability, and effects of spin-orbit interaction in semiconductors. Those students will gain essential knowledge on semiconductor physics, atom-atom interaction, spin physics, and density functional calculations.

Fu has experience working with more than ten undergraduate students, REU students in summer, and high-school teacher.

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