Research Areas and Lead Investigators
Chemistry Department

Dr. Xinle Li. The research group focuses on the development of crystalline porous materials, covalent organic frameworks (COFs), and their derived composites for energy and environmental applications such as heterogeneous catalysis, water remediation as well as a green synthesis of crystalline porous materials. The group develops a versatile synthetic toolkit for producing new COFs through integrated synthesis, characterization, application, and simulation feedback loops, which enables transformative research at the interface of COF chemistry, polymer science, organic material crystallization, computational simulations, and energy/environmental applications.

Dr. Conrad Ingram. Rare-earth perovskites ABO_3, particularly the orthoferrites $RFeO_3$ extensively investigated by the Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM), have garnered a surge of interest in 2D layered oxide materials synthetic availability, structural flexibility, unique ferroelectric, and ferromagnetic properties. The group uses the as-yet-unexplored assembly of 2D COFs on layered ABO_3 driven by lattice matching and interlayer interaction between adjacent layers, which is expected to create a new paradigm for ferromagnetic van der Waals heterostructures. The capability to synthesize, theorize, and tailor ABO_3/COF heterostructures with atomic precision will advance the underlying understandings of heterostructure formation and emergent ferromagnetic properties. Moreover, the marriage of ABO_3 and 2D COFs will produce a wealth of advanced ferromagnetic heterostructures that synergistically merge the merits of these constituent 2D materials, including atomic-level modularity, enormous structural flexibility, well-ordered structures, ferromagnetic character, and nontrivial optoelectronic properties, which will unleash the immense potential of ABO_3/COF ferromagnets toward spintronic applications.

Dr. Issifu Harruna. Graphene, a two-dimensional gapless semiconductor with a π-conjugated network, has intriguing electronic, thermal, and mechanical properties. The high aspect ratio of graphene and graphene nanoribbons (GNRs) offers an unprecedented opportunity for nanoscale functional interfaces that have potential applications in electronics, sensors, spintronics, and nanoelectronics. The group develops materials that combine the desirable properties of graphene and GNRs with the ease of processability of polymer-metal terpyridine complexes and their inherent photophysical properties. Hence, the properties of the designed materials can be manipulated by the careful choice of the metal ions and the polymer backbone. Therefore, providing a “toolbox” for the formation of desirable materials synergistically combining the characteristic features of metal centers and ligands. It is expected that these novel materials serve as fluorescence probes for diagnosis and other applications.

Dr. Eric Mintz. The research group’s goal is to develop 100% bio-based biodegradable composites which can compete with non-sustainable petroleum-based composites based on performance and cost. The group has a successful background in preparing lignin coated nanocellulose/poly(lactic acid) (L-CNC)/(PLA) composites by high torque melt mixing and extrusion that exhibit excellent processing and thermomechanical properties. Many polymers in use today, including petroleum-based polymers, incorporate fillers to improve material properties such as toughness, strength, and use temperature. These polymer/filler systems are referred to as composites materials, or composites. The use of nanomaterials, such as nanoclays, carbon nanotubes, and nanoparticles, as fillers has been expanding in recent years due to the vast improvement in material properties afforded by these nano-fillers. Unfortunately, these polymers and fillers are derived from unsustainable sources, such as petroleum and mining. Consumers, industry, and governments are increasingly demanding products made from renewable and sustainable resources that are biodegradable, non-petroleum based, carbon neutral, and have low environmental, animal/human health, and safety risks. Several bio-based biodegradable polymer systems have been developed, such as PLA, poly-3-hydroxybutyrate (PHB), and higher polyhydroxyalkanoates (PHA). However, these biodegradable bio-based polymers need reinforcement with fillers to be processed into composites that meet the rigors of applications in consumer goods.

Dr. Seyhan Salman. The research group focuses on the investigation of structural, electronic, and optical properties of organic pi-conjugated molecules and polymers for applications in new-generation organics-based semiconducting devices, such as organic light-emitting diodes (OLEDs), photovoltaic components, field-effect transistors, or chemical and biological sensors. For this purpose, the group uses a combination of theoretical models and computational approaches by bridging quantum chemistry, molecular dynamics, condensed matter and device physics, data science, materials and polymer science. This blended approach allows the researchers to discover and exploit multidisciplinary connections to enable new understanding that can be transitioned across several materials classes. The research is highly interdisciplinary and involves partnership with academia and industry. The group works closely with organic synthetic chemists and device engineers to develop new and innovative materials for organic electronics. Some of the ongoing research projects at the group are as follows: ♦ Fundamental Insight of Charge Transport in Organic Electronics. ♦ Electroluminescence in Solid-State Lighting and Display Technologies. ♦ Using High Performance Computing and Machine Learning Tools to Develop Fullerene-Free Acceptors for Organic Solar Cells. ♦ Fundamental Understanding of Interface Properties. Organic Bio-electronics.

Dr. Ishrat Khan. The proposed project aims to develop fundamental knowledge necessary to design next-generation advanced materials with the consideration of end-of-life features, i.e., multiple uses of advanced polymer and polymer composites. The group focuses on polymers with applications in electronic materials. The projects synergistically integrate experimental and computational studies to develop a structure-property-reactive-chemistry interrelationship to enable the effective design of the functional polymeric structures and advanced materials for high density energy storage. Using this approach, the researchers have successfully developed a polymer electrolyte with the highest known conductivity for application in lithium-air (LAB) and lithium-ion (LIB) batteries. All the projects include computational, synthesis and characterization. Advanced materials are characterized by the instrumentation available in our Core Research Facility which includes XPS, NMR, SIMS, GPC, DLS, AFM, SEM, XRD, and FTIR. Theoretical work includes the development of many-body perturbation theory based on the GW method and the variational Monte Carlo algorithm and applying the methods to the reactive mechanism of the polymeric networks.