Center for the Advancement of Topological Semimetals (CATS)
EFRC Director: Robert McQueeney
Lead Institution: Ames Laboratory
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***Mission Statement**: To discover and understand new magnetic topological materials that host quantum phenomena and functionality for future applications in computing, spin-based electronics, and sensing.*

Recent theoretical predictions and experimental discoveries of topological semimetals (TSMs), an entirely new class of materials, are opening an exciting frontier of science at the intersection of magnetism and topology. TSMs are poised to trigger breakthroughs in dissipationless spin and charge transport, such as high temperature quantum spin Hall and quantum anomalous Hall effects. Special TSMs, called Weyl semimetals (WSMs), can host extreme magnetotransport and optical properties, optically and magnetically switchable states. Understanding the basic principles of TSMs may also deliver new materials platforms for mid-infrared photodetection, night vision, and light harvesting. Research in this incipient field is fueling enthusiasm that TSMs will ignite transformational opportunities in spintronics, optoelectronics, quantum sensing, and classical (Beyond Moore's Law) and quantum computing.

To realize this potential, we (CATS) aim to discover and understand the properties of *magnetic* topological materials, including*;* magnetic TSMs, as well as magnetic WSMs, magnetically proximitized Dirac semimetals (DSMs), and two-dimensional (2D) spin-polarized DSMs. Magnetic TSMs provide the exciting potential of harnessing magnetic fields and magnetic interactions to control the flow of both charge and spin and their interconversion. We are developing methods to assemble atomically thin 2D layers and thin films of TSM into heterostructures with other magnetic materials to deliver functionality and even induce new topological states of matter. The basic principles for the control and manipulation of TSM functionalities are being unveiled by studying the interaction of TSM materials with external fields.

With leading expertise in the theory of TSM, new materials discovery, the assembly of heterostructrures, and advanced characterization methods, CATS is advancing our understanding and accelerating breakthrough innovations in TSMs. CATS pursues **three integrated, fundamental research goals** that address essential issues in TSM research:

1. *Predict, discover, and understand archetypal magnetic TSMs and new magnetic topological states-of-matter.* There is a need to discover new magnetic TSM compounds with simpler topology and the absence of trivial bands near the Fermi energy. Also, the combination of TSM with other materials in heterostructures can deliver new quantum topological states. CATS addresses these materials challenges with a systematic approach described below.
2. *Controllably induce topological phase transitions.* An important milestone for CATS is a clear demonstration that topological properties can be controlled. This requires the ability to create, modify, or annihilate the topologically protected electronic states. CATS uses a multitude of methods to enable TSM control, such as carrier doping, electrostatic gating, magnetic fields, strain and dimensionality (in thin films), and proximity effects (in heterostructures).
3. *Manipulate the response of topological states to external fields.* Demonstrating that TSM states can be manipulated is the first step toward fulfilling their promise in information and sensing technology. One route to achieve this goal is to take advantage of gapless topological bands and utilize their unique light-matter and optoelectronic responses to manipulate and switch charge/spin currents or to generate collective electronic effects. CATS researchers exploit the unique pulsed high magnetic fields and ultrafast coherent photon excitations to manipulate TSMs and potentially discover new states of matter.

To attain these goals, CATS employs innovative approaches that are organized into **three crosscutting research thrusts (RTs) to**: **(1) predict, discover, and understand new bulk magnetic TSMs; (2) discover and control novel quantum states and functionality in thin films and heterostructures; and (3) investigate the dynamical manipulation of topological states.** The goals and RTs of CATS are interwoven. For example, the discovery of new topological states of matter (Goal 1) may be discovered in bulk single crystals (RT-1) or heterostructure assemblies (RT-2), or under non-equilibrium conditions in applied fields (RT-3). In addition, the development of emergent functionality in layered heterostructures of 2D materials (RT-2) requires the discovery of new, exfoliatable TSMs (RT-1).

Developing the unique functionalities of TSMs is a *complex materials challenge.* CATS discovers archetypal TSM compounds and delivers high-quality, well-characterized materials to be used as building blocks in heterostructures. All research thrusts in CATS exploit premier synthesis and characterization capabilities and the ability to apply static and time-dependent external fields to manipulate and switch TSM properties. CATS combines fundamental theory and insight with first-principles electronic structure calculations; results from such calculations for relevant materials and heterostructures will be used to construct response functions, magnetotransport models, and non-equilibrium theories. CATS also utilizes DOE-supported neutron sources, light sources, nanocenters, and leadership computing user facilities.

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