Energy Frontier Research Centers

Quantum Information Science Awards Abstracts

Programmable Quantum Materials (Pro-QM)
Energy Frontier Research Center
Director: Dmitri Basov, Columbia University
Co-PIs: Cory Dean (Columbia), James Hone (Columbia), Michal Lipson (Columbia), James Shuck (Columbia), Andrew Millis (Columbia), Abhay Pasupathy (Columbia), Xiaodong Xu (U. Washington), David Cobden (U. Washington), Daniel Gamelin (U. Washington), Jiun-haw Chu (U. Washington), Di Xiao (Carnegie Melon)

The Institute for Quantum Matter (IQM)
Energy Frontier Research Center
Director: Collin Broholm, Johns Hopkins University (JHU)
Co-PIs: N. Peter Armitage (JHU), Robert Cava (Princeton), Natalia Drichko (JHU), Seyed Koohpayeh (JHU), Yi Li (JHU), Tyrel M. McQueen (JHU), Satoru Nakatsuji (Tokyo/JHU), Predrag Nikolic (George Mason/JHU), Brad Ramshaw (Cornell), Nitin Samarth (PSU), Oleg Tchernyshyov (JHU), and David Vanderbilt (Rutgers)

Center for Molecular Magnetic Quantum Materials (M2QM)
Energy Frontier Research Center
Director: Hai-Ping Cheng, University of Florida (U. Florida)
Co-PIs: Garnet Chan (Cal Tech), George Christou (U. Florida), Arthur Hebard (U. Florida), Richard Hennig (U. Florida), Stephen Hill (Florida State), Talat Rahman (U. Central Florida), Neil Sullivan (U. Florida), John Stanton (U. Florida), Samuel Trickey (U. Florida), Vivien Zapf (Los Alamos National Laboratory), Xiaoguang Zhang (U. Florida)

Center for Novel Pathways to Quantum Coherence in Materials (NPQC)
Energy Frontier Research Center
Director: Joel E. Moore, Lawrence Berkeley National Laboratory (LBNL)
Co-PIs: James Analytis (LBNL), Elke Arenholz (LBNL), Stefano Cabrini (LBNL), Michael Crommie, Peter Ercius (LBNL), Naomi Ginsberg (LBNL), Alessandra Lanzara (LBNL), Jeffrey Neaton (LBNL), Joseph Orenstein (LBNL), Ramamoorthy Ramesh (LBNL), Eli Rotenberg (LBNL), Feng Wang (LBNL), Chao Yang (LBNL), Norman Yao (LBNL), David Awschalom (ANL; Deputy Director), Aashish Clerk (ANL), Giulia Galli (ANL), Supratik Guha (ANL), F. Joseph Heremans (ANL), Martin Holt (ANL), Jiwoong Park (ANL), Xufeng Zhang (ANL), Dmitri Basov (Columbia), Ania Bleszynski Jayich (U. Cal Santa Barbara)

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Co-Investigators: Columbia University: Cory Dean, James Hone, Michal Lipson, James Shuck, Andrew Millis, Abhay Pasupathy. University of Washington: Xiaodong Xu; David Cobden, Daniel Gamelin, Jiun-haw Chu. Carnegie Melon: Di Xiao
https:\\quantum-materials.columbia.edu

Quantum materials (QMs) manifest the many roles of topology, dimensionality and strong correlations in defining macroscopic observables. The vision for this Energy Frontier Research Center on Programmable Quantum Materials is to discover and deploy new forms of quantum matter controllable by external stimuli, atomic-layer assembly, magnetic proximity, and nanomechanical manipulation, with the goal of effectively programming their quantum properties.

The particular materials systems we will focus on are the transition metal dichalcogenides (TMDCs) and 2D-halides, two large classes of layered van der Waals (vdW) solids combining a vast range of properties with an unprecedented degree of controllability. The key novelty of the Pro-QM approach is developing strategies for transforming QMs into desired states with tailored quantum properties not attainable in common metals or semiconductors. In parallel, we will investigate the formation of on-demand macroscopic coherent states. Pro-QM will engineer coherent phenomena and robust quantum fluids formed by excitons and exciton-polaritons in vdW heterostructures. The research objectives rely on two cross-cutting themes: *i)* creation of new tailored materials and architectures hinging on combinations of vdW atomic layers assembled in complex heterostructures; and *ii)* transformative advances in experimental imaging tools for probing optoelectronic and magnetic properties at native length- and time-scales.

This ambitious program calls for an outstanding team with diverse and complementary expertise. Our team combines emerging (untenured) leaders together with senior researchers with extensive track records of collaborative and impactful research underpinning the field. Guided by concrete and compelling scientific goals and technical approaches, this team will act as cohesive squad in which all members have well defined roles.

The impact. The goals of Pro-QM EFRC are daring in their experimental and intellectual reach, and promise disruptive impact on a range of Grand Challenges for fundamental energy research. A concerted EFRC effort is imperative for making the desired leaps. Every element of the Pro-QM program is related to novel ways of controlling, detecting, processing and transmitting information in complex structures in fundamentally new and energy efficient ways, an outcome with major societal impact.

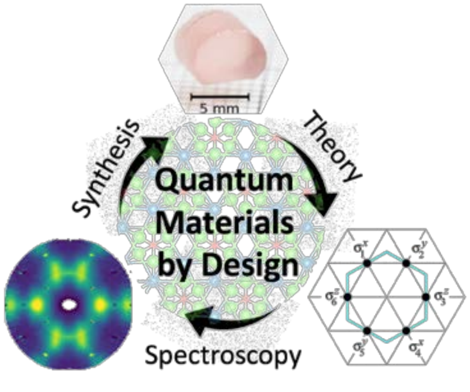
The Institute for Quantum Matter (IQM) Energy Frontier Research Center

Collin Broholm (EFRC Director, Johns Hopkins U.), N. Peter Armitage (JHU), Robert Cava (Princeton), Natalia Drichko (JHU), Seyed Koohpayeh (JHU), Yi Li (JHU), Tyrel M. McQueen (JHU), Satoru Nakatsuji (Tokyo/JHU), Predrag Nikolic (George Mason/JHU), Brad Ramshaw (Cornell), Nitin Samarth (PSU), Oleg Tchernyshyov (JHU), and David Vanderbilt (Rutgers)

The discovery and characterization of quantum materials is one of the grand challenges of 21st century physical science. New materials, developed though a deep understanding of their underlying physics, will play an essential role in extending the information technology revolution and confronting the unprecedented growth in global energy needs. Despite many important advances, quantum materials continue to present deep fundamental challenges. How can we predict and control the collective properties of 10^{23} electrons in a solid? What novel quantum dominated states of matter, and electronic and magnetic properties may ensue? The opportunities for fundamental discoveries that could transform technologies are bountiful as we extend our ability to understand and control collective quantum phenomena in materials.

The Institute for Quantum Matter Energy Frontier Research Center consists of a collaborative team of scientists that spans the materials-by-design triad of materials discovery and synthesis (single crystals and thin films), advanced experimentation (neutron scattering, optical spectroscopies, transport, ultrasound, and high magnetic field techniques) and theory (analytical and numerical). The Institute is pursuing four types of quantum matter that have not previously been realized: **Topological magnetic semimetals, quantum spin liquids, monopole superconductors, and axion insulators.** Each target presents distinct challenges with deep intellectual connections. There are also crosscuts between areas in terms of the techniques and methods used so that successes in one area advance others.

As we make progress in the realization and characterization of quantum materials, their unique physical properties present opportunities for breakthrough applications in energy and information. These include practical superconductivity for energy storage and distribution, materials with emergent quantum coherent particles for quantum information processing, systems that afford the possibility to control magnetic degrees of freedom with electrical drive, and new platforms for energy efficient electronics. IQM is motivated by the fundamental challenges that correlations and topology present but as our understanding of interacting electrons progresses, we shall also bring the application potential of quantum materials into focus.



The IQM mission: To realize, understand, and control revolutionary quantum materials and structures where quantum effects such as entanglement and coherence find collective macroscopic manifestations.

Center for Molecular Magnetic Quantum Materials (M2QM)
Energy Frontier Research Center

Director: Hai-Ping Cheng[1]
Co-PIs: Garnet Chan[2], George Christou[1], Arthur Hebard[1], Richard Hennig[1], Stephen Hill[3], Talat Rahman[4], Neil Sullivan[1], John Stanton[1], Samuel Trickey[1], Vivien Zapf[5], Xiaoguang Zhang[1]
[1]University of Florida, [2]California Institute of Technology, [3]Florida State University, [4]University of Central Florida, [5]Los Alamos National Laboratory

Cloud computing and ultra-high performance computing consume enormous amounts of electrical power cooling the machines. The ones and zeros of binary arithmetic are switched physically by moving electrons through circuits. Moving these electric charges with an electric field consumes power. When billions of circuits all move electrons in a modern computer, there is an enormous power consumption, hence enormous waste heat. But what if we could represent the binary numbers with some sort of switchable physical phenomenon that does not require moving charges in an electric field and thus reduce heating? Magnetic hard drives use switchable magnetic polarization (up and down) to store digital bits. Switching magnetic polarization does not require moving any charge. But magnetic memory devices are difficult to integrate into a circuit, because reading and writing the bits usually requires applying a magnetic field. The central quest of the M^2QM project is to achieve this magnetic switching at the scale of molecules and allow switching and reading with an electric field.

Multiple challenges exist. Magnetism is a quantum mechanical property. That leads to the concept of "quantum materials". These are materials in which quantum mechanics is important not just for holding the material together and giving it properties (metal or semiconductor, hard or soft, etc.), but also for being the fundamental origin of usable atomic-scale phenomena. Our study of quantum materials is focused on a wide variety of inter-connected interactions, including magnetic interactions, magnetoelectric interactions and molecule-substrate interface interactions, in a new class of magnetic molecular quantum compounds and in a large group of materials that are made of single-molecule magnets. Both groups contain transition metal atoms as the magnetic centers. These materials can exhibit simultaneous changes in the crystal structure, the electric polarization, and magnetization, making them good candidates for electromagnetic manipulations. This property has the name of "multi-ferroic" materials. In a conventional material, application of an electric field changes the polarization. In a multi-ferroic, this change then in turn changes the magnetic state. Clearly multi-ferroism is a route to electrically switch a magnetic molecule.

The eight theorists and computationalists on the M^2QM team, equipped with a nearly complete computational toolbox and working in close collaboration with experimentalists, will build models to simulate spin state control and multi-ferroism and investigate key approximations for accuracy. The four experimenters will synthesize magnetic molecules and characterize them, then assemble them onto substrates and probe their controllability and responses. This research will go a long way to answering two key Department of Energy questions: "*How do we control material processes at the level of electrons?* and "*How do we design and perfect atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties*?" M^2QM thus will lay the ground work for molecular magnetic quantum materials for advanced, low-power digital devices.

Center for Novel Pathways to Quantum Coherence in Materials (NPQC)
Energy Frontier Research Center

Director: Joel E. Moore, Lawrence Berkeley National Laboratory (LBNL)

LBNL: James Analytis, Elke Arenholz, Stefano Cabrini, Michael Crommie, Peter Ercius, Naomi Ginsberg, Alessandra Lanzara, Joel Moore (Director), Jeffrey Neaton, Joseph Orenstein, Ramamoorthy Ramesh, Eli Rotenberg, Feng Wang, Chao Yang, Norman Yao
ANL: David Awschalom (Deputy Director), Aashish Clerk, Giulia Galli, Supratik Guha, F. Joseph Heremans, Martin Holt, Jiwoong Park, Xufeng Zhang
Columbia: Dmitri Basov
UCSB: Ania Bleszynski Jayich

This Energy Frontier Research Center for Novel Pathways to Quantum Coherence in Materials will dramatically expand our understanding and ability to control coherence in solids by building on recent discoveries in quantum materials along with advances in experimental and computational techniques. Common threads are the need to understand defects in complex material environments, the use of high-resolution optical techniques and other cutting-edge experimental tools, and the role of inhomogeneity in various types of quantum materials. The first thrust of research involves point defects in simple and complex insulators and the improvement of their coherence properties for potential uses such as quantum sensing of temperature, magnetic fields, and local strain and electric fields.

The second thrust builds on recent discoveries in interfaces and boundaries of two-dimensional materials, in order to understand coherent one-dimensional conduction with the potential to avoid dissipation and heating. These unique “quantum wires” can serve as interconnects for quantum information.

The third thrust aims to understand and enhance linear and nonlinear electrodynamic responses in topological, magnetic, and other highly correlated quantum materials, using advanced coherent methods to elucidate the role of static and dynamic fluctuations at short length scales. In addition to possibly providing alternatives for solid-state quantum computation, strongly correlated materials such as these are one of the key science drivers that the first quantum computers will be used to attack. *Progress in these thrusts will enable new solid-state approaches to quantum sensing, communication, and computation.* Improved understanding of the quantum materials under study will also impact more conventional electronic and optical applications by demonstrating new materials for switchable and nearly dissipation less transport, single-pass frequency doubling, and efficient terahertz detection.

Research will be carried out at four institutions (LBNL, ANL, Columbia, and UCSB) by an integrated team of experimentalists and theorists, taking advantage of the unique facilities available at the national laboratories.