

Design and Synthesis of Materials for Low-Mass Dark Matter Detection and Sensing

Thematic Areas:

(TF10) Quantum Information Science.

(TF9) Theory Frontier: Astroparticle

(CF1) Cosmic Frontier: Dark Matter: Particle Like

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Model of dark matter (DM) that assign DM mass to the sub-GeV range have opened up the prospect of using low-energy excitations in solid-state materials as low-mass detector targets. Several condensed matter systems have been already explored for such low-mass detection including scintillators, Dirac materials, superconductors, polar materials and superfluid helium¹⁻⁶.

Many of these approaches rely on DM coupling to single-particle and collective excitations such as electron-hole generation, and magnon and phonon excitations^{5,7,8}. Recent work carried out a comparison of commonly-used semiconductor detector targets to optimize reach to electron- and phonon-DM scattering and absorption^{9,10}. However, the optimal target material for each of these detection modes is not yet known – both readout schemes and additional target features such as directionality can be included as additional constraints on target selection^{9,11,12}.

Parallel to the push to lower-mass target development has been the recent strides in quantum materials with the discovery of novel correlated phases and phenomena that include spin, topology and orbital degrees of freedom. However, current sensors and detectors do not yet take advantage of the thriving field of correlated quantum phenomena and materials where small perturbations can result in threshold or cascade events, apt for small mass/energy detection.

In this LOI, we propose solid-state physics approaches to low-mass DM detection with the following two themes:

I. MATERIALS BY DESIGN FOR OPTIMAL TARGETS

Materials theory and design is now facilitated by the huge advances in accurate materials modeling and supercomputing power. Such methods have made key discoveries and advances in fields as disparate as multiferroics, superconductivity and photovoltaics. We propose expanding and optimizing the design of new quantum materials for DM detection. To do this we will combine symmetry considerations, first-principles calculations based on density functional theory (DFT) and related electronic structure methods and high-throughput materials informatics with databases such as the Materials Project^{13,14}. With these methods we can elucidate structure-property relationships to develop models and design rules with the aim of detection and readout enhancement by physical and chemical tuning. Our material predictions can then be used as a guide for the synthesis of optimal sensor and detector materials, with a theory/experiment feedback loop for improved predictions and synthesis. Two examples where this approach can be used are proposing anisotropic materials, using a combination of materials-by-design and high-throughput materials informatics, and in combined target/readout schemes for optimal detector design.

II. CORRELATED METASTABLE QUANTUM MATERIALS FOR LOW-MASS DETECTION

Correlated quantum materials with spin, orbital and topological degrees of freedom often have competing ground states that are close in energy¹⁵. This proximity to multiple energy states makes them apt for exploring detection and sensor events for low-threshold phenomena. For instance threshold and cascade phenomena have been observed in transition metal dichalcogenides such as 1T-TaS₂ where transitions between metastable states can be driven by small perturbations¹⁶. A key advantage to this is insensitivity to defects; in traditional target proposals crystalline and other defects are detrimental to target performance, however many of these correlated quantum systems are robust against defects, and are often a feature. This second topic aims to explore new detection regimes using the collective,

correlated phenomena in quantum materials – it will investigate the landscape of metastable ground states which can be driven by small perturbations, and relate their energy scales to sensitivity estimates for low-mass DM.

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