

Plan Overview

A Data Management Plan created using DMPTool

Title: FRG20

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Project abstract:

NiS(2-x)Se(x) as a model system for insulator-to-metal transition (IMT) is proposed in this work. NiS(2-x)Se(x) is considered as a classical model for NiS₂ Mott insulator with Se substitution. The advantage comes as the end crystals, NiS₂ and NiSe₂ are insulator and metallic, respectively, and they have the same pyrite crystal structure. Thus, one might expect the evolution toward metallicity comes from changing the ionic radii of the dichalcogenides, leading to stronger p-d hybridization, with no crystallographic complexity. Despite the long-term study of NiS(2-x)Se(x), understanding IMT puzzles researchers, and discrepancies in results have been reported in magnetic and electronic properties. Thio et. al postulated strong surface conduction that controls the transport properties at low temperature. FeS₂ has recently gained attention as an alternative source for photovoltaic applications. FeS₂ is unfortunate with low open circuit voltage that limits solar-to-electric power efficiencies. Magnetoresistance and Hall in as-grown single crystals showed that FeS₂ is contaminated with two-dimensional (2D) conductive surface layer. The layer hinders the carrier of the bulk, effort nowadays is trying to understand and passivate the layer which will introduce progress to FeS₂ as conversion devices. Transport on NiS₂ show the existence of 3 nm 2D layer, and with Se substitutions, we propose to study the evolution of the 2D layer with the IMT. This introduces major modification to the longed-believed phase diagram of NiS(2-x)Se(x) that was illuded by 2D layer. We propose to grow single crystals NiS_{2-x}Sex by chemical vapor transport (CVT) method in range $0 \leq x \leq 1$, in 0.1 step, transport, and magnetic properties will be investigated by Physical Properties Measurement System (PPMS) which is available at the Materials Science Laboratory at AUS. This work lies at the heart of the PI expertise and his experience in the topic of magnetism and magnetic materials. The PI spent his graduate school, post-doctoral, and currently since 2010 at AUS investigating magnetic properties of strongly correlated electron systems using profound techniques. This fund goes to get high-quality single crystals, training students, mediating discussion with experts, conducting an experiment at NIST and UMN, and presenting data in well-known conferences such as the MMM series.

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Data will be collected at Materials science and Engineering research laboratories using Physical Property Measurement System to measure transport and magnetic properties of $\text{NiS}(2-x)\text{Se}(x)$ single crystals.

Data will be saved on data acquisition computer and will be backed up regularly using external hard drive.

There are no privacy requirements, data and analysis will be available to people in the materials laboratory.

Data will be shared internally to students and the PI. Data will be presented in conferences in a discussion way and exchanging ideas in preparation final version.

Data will be localized in PPMS computer and external hard drive with proper name and directory that are easy to access in the future.

Backing up data on different computers and external memories.
