

---

## Plan Overview

*A Data Management Plan created using DMPTool*

**Title:** FRG20

**Creator:** Sami El-Khatib

**Affiliation:** American University of Sharjah (aus.edu)

**Funding opportunity number:** 46098

**Template:** Data Management Plan - AUS Funded Research

### 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 NiS<sub>2</sub> Mott insulator with Se substitution. The advantage comes as the end crystals, NiS<sub>2</sub> and NiSe<sub>2</sub> 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. FeS<sub>2</sub> has recently gained attention as an alternative source for photovoltaic applications. FeS<sub>2</sub> is unfortunate with low open circuit voltage that limits solar-to-electric power efficiencies. Magnetoresistance and Hall in as-grown single crystals showed that FeS<sub>2</sub> 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 FeS<sub>2</sub> as conversion devices. Transport on NiS<sub>2</sub> 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<sub>2</sub>-xSex 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.

**Last modified:** 10-20-2019

### Copyright information:

The above plan creator(s) have agreed that others may use as much of the text of this plan as they would like in their own plans, and customize it as necessary. You do not need to credit the creator(s) as the source of the language used, but using any of the plan's text does not imply that the creator(s) endorse, or have any relationship to, your project or proposal

## FRG20

---

### Data Collection

**Give a summary of the data to be collected or produced.**

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

### Storage and Back-up

**How will the data (digital or non-digital formats) be stored and backed up during the research?**

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

### Access and Use Rights

**What steps will be taken to protect privacy, confidentiality, intellectual property or other rights?**

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

### Sharing Data and Controlling Access

**Will data be shared during the course of the project?**

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 Organization, Documentation and Metadata

**What documentation and / or metadata (information about the data) will ensure data can be retrieved and used?**

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

### Data Preservation and Archiving

**Should the data be considered for permanent retention / archiving?**

Backing up data on different computers and external memories.