Research Statement: Present and Future

As an experimental condensed matter (solid state) physicist, my main interests reside in investigating the fundamental properties of materials that have potential technological applications. Specifically, I am interested in studying the role and impacts of impurities in a variety of semiconductors and their optical, electrical and magnetic properties. My interests also reside in developing a higher understanding of the fundamental mechanisms that give rise to phenomena such as heavy fermion behavior, magnetic frustration, various types of magnetic order and transitions (e.g.: metal to semiconductor/insulator, magnetic, superconducting, optical).

My current work primarily uses the Muon Spin Research technique (MuSR) which implants 100% spin polarized muons (μ^+: $q = +e$; $\gamma_\mu = 135.54\frac{MHz}{T}$; $\boldsymbol{S} = \frac{1}{2}$; $m_\mu = \frac{1}{9}m_p$; $\tau{\sim}2.2\mu s$) in a material to map the local electronic and magnetic environment [1]. Due to its similarities to a proton and relatively large magnetic moment, μ^+ serves as both an experimentally accessible analog to the early time history of hydrogen impurities in semiconducting and insulating materials in addition to a very sensitive probe to the local magnetic environment. My work also requires a variety of electrical, magnetic and optical characterization techniques; most of which is available at the national laboratories where the MuSR experiments are conducted or I intend to build in a local characterization laboratory. This work also involves a significant amount of modelling and simulation work to supplement the MuSR data.

As an example, my Ph.D. research investigated the local magnetic environment of II-IV-V_2 chalcopyrite dilute magnetic semiconducting (DMS) systems, using MuSR, neutron scattering and bulk magnetic characterization techniques. Some of the II-IV-V_2 chalcopyrites show room temperature ferromagnetism when weakly doped with Mn while maintaining their semiconducting properties, which makes them ideal candidates for spin-electronics applications. Conventional models for magnetism in DMS such as *double-exchange* for III-V materials (i.e. GaAs:Mn, GaP:Mn) or *indirect [Zener] exchange* for II-VI materials (i.e. CdTe:Mn) fail to explain the observed ferromagnetic features in the II-IV-V_2 systems as these models require either a much higher carrier concentration or magnetic ion content than *actually* needed for the II-IV-V_2 chalcopyrites. The main open question my Ph. D. project addresses is how the magnetism in weakly Mn-doped II-IV-V_2 chalcopyrites is mediated from the local Mn impurities throughout the bulk material in order to help establish a model relevant to the II-IV-V_2 DMS systems. Results from this project show that spin polarons provide the transfer of magnetism from the local moments (Mn) to the charge carriers (holes, in this case) in the weakly doped II-IV-V_2 chalcopyrite systems thereby providing the basis for a model that can explain the observed magnetic properties. [2]

After my Ph.D., I have started a series of new projects. One of my current projects is focused on studying the dynamics and stability of Hydrogen impurities in the rutile, anatase and brookite phases of Titanium Dioxide (TiO_2) [3]. TiO_2 is of considerable interest for use in applications such as gas sensing systems, H storage, electrochromic devices and is under consideration as a replacement to SiO_2 as a gate oxide material in highly miniaturized transistors [4]. While the rutile phase is currently the most prevalent, the anatase phase is the most active in several of these applications and its activity is enhanced by the addition of H impurities. Moreover, the electrical properties in all three phases are significantly different. While the effects of H incorporation on the bulk materials have been studied, the actual role H plays in modifying the system is still an open question. Our group has made considerable progress on understanding the behavior of H in rutile TiO_2 via MuSR as we have identified that ground state configuration for Muonium ($Mu=\mu^+ + e^-$) is composed of a μ^+ adjacent to an O and coupled to an e^- that is centered on a neighboring Ti^{3+} (small polaron) opposed to a true effective mass donor state [3]. We have completed a round of experiments on both anatase and brookite TiO_2 where the low temperature behavior in each also suggests a similar state to what we find in rutile. We have additional

MuSR beamtime approved and scheduled for a detailed follow up to work out the motional and charge-state dynamics in all three phases. This should provide a significant contribution to understanding the role that H impurities play in modifying the electrical properties of these materials, which is essential in promoting meaningful and efficient technological developments. I presented preliminary findings of this work at the 14th International Conference on Muon Spin Rotation, Relaxation and Resonance in June 2017, held in Sapporo, Japan and additional progress at a Gordon Research Conference focused on defects in semiconductors in August 2018.

Another of my current projects investigates magnetism and properties of the early time history of Hydrogen impurities in Vanadium Dioxide (VO_2) compounds. Stoichiometric VO_2 exhibits a reversible metal-semiconductor transition (MST) where it is metallic above T_{MST} (≈ 340K) and semiconducting below T_{MST}. A structural transition accompanies the MST and both are triggered by thermal, optical, electrical or barometric means. Considerable disagreement regarding the mechanism(s) responsible for these ultrafast ($t\sim10^{-12}$ –10^{-3} [s] timescale) transitions still exist, despite being studied for decades. Some donor and acceptor impurities change T_{MST} without significantly modifying the electronic, optical or switching properties. The *effects* that a variety of impurities have on the material properties are well known, however, the *role* they play in modifying them is far from understood [5]. I am using *MuSR* and *neutron scattering* techniques to characterize the newly discovered (by us) low temperature magnetic phase [6], the MST and how properties therein are modified by the presence of impurities such as H, W and Ti with the overall goal of developing a better understanding the fundamental mechanism(s) that drive the transitions.

I am also interested in developing new experimental techniques. I have been active in working with instrument scientists at Rutherford Appleton Lab in the development of a brand new MuSR experimental technique on semiconductors that uses a combination of traditional muon spectroscopy with a wavelength tunable laser to perform direct spectroscopic measurements of the Muonium donor levels, acceptor levels and vibrational states. This is opening a wide range of new possibilities in understanding the Mu (H-like) impurity, photocarrier interactions and stimulated dynamics of a host.

Some examples of other projects in which I am leading or actively involved are studying the Mu (H) behavior in several classes of semiconducting materials with applications (such as the Transparent Conducting Oxides, Wide-gap Oxides, SiGe alloys).

Long-term, I plan to continue investigating the role and effects impurities have in modifying the electrical, magnetic and optical properties of new materials with potential applications. These studies will require magnetic, electrical and optical characterizations that I intend to setup in a local characterization laboratory and supplement with accelerator-based experiments, such as MuSR. Additionally, I hope to be able to use my expertise with the MuSR technique to supplement existing work within any department that I have the privilege to join, as it is a versatile and novel tool with the ability to probe length and time scales of local environments not easily available by other techniques.

[1] See e.g.: S.J. Blundell, *Contemporary Physics* **40** (1999) 175; J.H. Brewer, in *Encyclopedia of Applied Physics*, ed G.L. Trigg (VCH, New York, 1994), **11** pp 23-53.
[2] P. W. Mengyan, Magnetism in Mn-Doped Chalcopyrites, *Ph.D. Dissertation* (2014) Texas Tech University;
P. W. Mengyan, et al., *AIP Conf Proc* **1583** (2014) 190.
[3] see e.g.: R.C. Vilão, *et al*., *Phys Rev B* **92** (2015) 081202(R)
[4] see e.g.: J. Zhang, *et al*., *Phys Chem Chem Phys* **16** (2014) 20382; X. Chen, *et al., Chem Rev* **107** (2007) 2891;
U. Diebold, *Suf Sci Rep* **48** (2003) 53.
[5] e.g.: M. Imada, et al., *Rev Mod Phys* **70** (1998) 1039; J.B. Goodenough, *J Solid State Chem* **3** (1971);
C. Wu, et al., *J Am Chem Soc* **133** (2011) 13798; P. Kira, et al., *Adv Mat Lett* **1** (2010) 86; Burkhardt, et al., *Thin Solid Films* **345** (1999) 229.
[6] P. W. Mengyan, et al., *J Phys: Conf Ser* **551** (2014) 012017