Research Statement and Future Plan

Overview

My scientific interests bridge the areas of Magnetism and Quantum (Topological) & Superhard Materials for novel Materials/Chemical Engineering applications and Smart Multifunctional Devices.

In particular, my research interests lie in the field of Advanced Magnetic Materials, Spectroscopy, and Nano-electronic Materials for spin-orbitronics, anti-corrosive applications, optoelectronics and optimized thermoelectric generators (thermoelectricity, magnetothermal etc.). My research will be focused on Mott insulators (MI)[1] and Topological Insulators (TI)[2,3,4] and the investigation of related subjects, such as interfacial phenomena, superconductivity, spintronics, TI surface states, thermo-electrics, and their relevant emergent phenomena and Chemical Engineering and Bioengineering applications (electronic devices and circuits).

Over the last ten years, I have applied various magnetic characterization techniques such as : Magnetic Resonance (NMR) and Nuclear Quadrupolar Resonance (NQR) techniques/methodology to the study of magnetic, superconducting, and structural phase transitions. Activities were focused in the study of colossal magnetoresistive perovskites (e.g. the $La_{1-x}Ca_xMnO_3$ family), superconducting materials such as cuprates, pnictides, transition metal borides, and magnetic nanoparticles. The synthesis and characterization of nanostructures constituting ferromagnetically soft/hard and antiferromagnetic layers, known as exchange bias for spintronics, were my main interests. My research experience amongst the experimental NMR procedures was focused on modern and conventional magnetic resonance techniques and methods such as the NMR probe design/construction and cryogenic instrumentation. In addition, electrochemical solid-state techniques were employed with emphasis in the study of micro and nano-coatings for industrial and naval anticorrosion engineering.

I have established several productive cross-disciplinary collaborations with universities and national laboratories (*e.g.*, NHMFL, Helmholtz-Zentrum Berlin) among which research with Northwestern University and TRIUMF at Canada are the two most recent efforts with projects funding from DARPA and several NSF proposals.

Recent Research Studies & Achievements

As a postdoctoral researcher at the University of California, Los Angeles (UCLA), my research dealt primarily with the investigation of Topological Insulators (TIs) and Thermoelectric (TEs) compounds. These studies involved production, characterization and understanding of novel phenomena and phase transitions in condensed matter systems arising from interfaces and heterostructures of TI/TE materials. My contribution involved developing and testing novel (solid-state) NMR, NQR and spin-polarized radioactive ion beam magnetic resonance techniques (μSR, β-NMR) and hardware development for the discovery of novel phases of matter. My overarching goal was to study novel physics (such as new phases of matter involving heterostructures of TIs, including Weyl semimetal[6]), study the effect of defects and impurities on the topologically protected states, with the ultimate goal of engineering the TI material for nanoelectronic applications. This entire project lasted for three years and involved extensive collaborations with groups at UCLA, Caltech, Stanford, UC Berkeley, Northwestern and TRIUMF at Canada.

During these years, I developed new NMR methodology to characterize bulk and surface states of binary and ternary chalcogenides[7-11]. The chalcogenides are renowned for their valuable topological insulating and the thermoelectric properties. One component of this project was a comprehensive (conventional) NMR investigation of the band structure and the density of states of V_2VI_3 layer-type chalcogenides. Prototype TE and TI compounds of my interest included antimony telluride (Sb_2Te_3), bismuth selenide (Bi_2Se_3) and bismuth telluride (Bi_2Te_3) as well as ternary chalcogenides (Bi_2Te_2Se, $Bi_{0.5}Sb_{1.5}Te$, $Pb_{1-x}Sn_xTe$ etc.). The second component of the project was a search for TI signatures in a depth-resolved manner by using thin films and nanocrystals. During this second part, I divided my time between UCLA and the national lab of particle and nuclear physics (TRIUMF) in Vancouver, where I worked as a visiting scientist in the μSR and β-NMR groups of Prof. Rob Kiefl and Prof. W.A. MacFarlane. During this period I performed a series of interesting experiments that included: a) β-NMR Studies of Topological Crystalline Insulator States, b) Study of Vacancy Defects in Topological Insulator via μSR, c) β-NMR Investigations of the Topological Magneto-Electric Effect, and d) β-NMR studies of the surface states of topological insulators. In many of these projects I collaborated with institutes from all around the world, including the University of British Columbia, Princeton, Paul Scherrer Institut, University of Texas, Austin and Northwestern University.

At TRIUMF, I have performed the first nuclear experiments on TI heterostructures, which lead to the first ever detection of an NMR signal from the TI surface states[12,13]. This discovery provides a way to use a large particle accelerator for visualizing properties of nanoscale electronic materials and has attracted considerable media interest[14-20]. At UCLA, I applied variable temperature and particle size dependent studies on topological insulators and topological crystalline insulators in order to detect the impact of the defects in the surface states by changing their surface-to-volume ratios[21] as well as investigating via NMR the Band Inversion effect[11].

Characteristics examples representing my research plans are as follows in the next two sections:

Research Interests

I. Design and Characterization of new Quantum and Magnetic Materials via advanced techniques (Theory and Experiment)

An ideal TI has a bulk interior characterized by an insulating band gap, while the boundary exhibits gapless Dirac-like edge (2D-TIs) or surface states (3D-TIs). The observation of metallic surface states often requires minimal bulk defects or compensation for the free carriers. Chalcogenides are an ample platform for this phenomenon. The discovery of topological insulators has changed the way we look at chalcogenides as the chalcogenides offer a desirable platform for investigation both thermoelectric and topological insulating properties. Additionally, these binary semiconductors revealed precious thermoelectric power and applications as solid-state power generators and refrigerators (Peltier, Seebeck and Thomson devices). An effort aimed at improving the TE efficiency (figure of merit parameter, *ZT*) concluded that Bi_2Te_3-Sb_2Te_3 solid solutions yield improved TE materials, according to the *ZT* parameter, which is maximized in $Bi_{0.5}Sb_{1.5}Te_3$. Other ternary telluride compounds in the same class as these layered materials, Bi_2Te_2Se and Bi_2Te_2S, show the potential of tuning and enhancing transport properties. However, the underlying physics that govern the TE efficiency is still not fully explored. Efforts will be made in order to combine both TE and TI properties in the same compound and to be identified microscopically by NMR measurements.

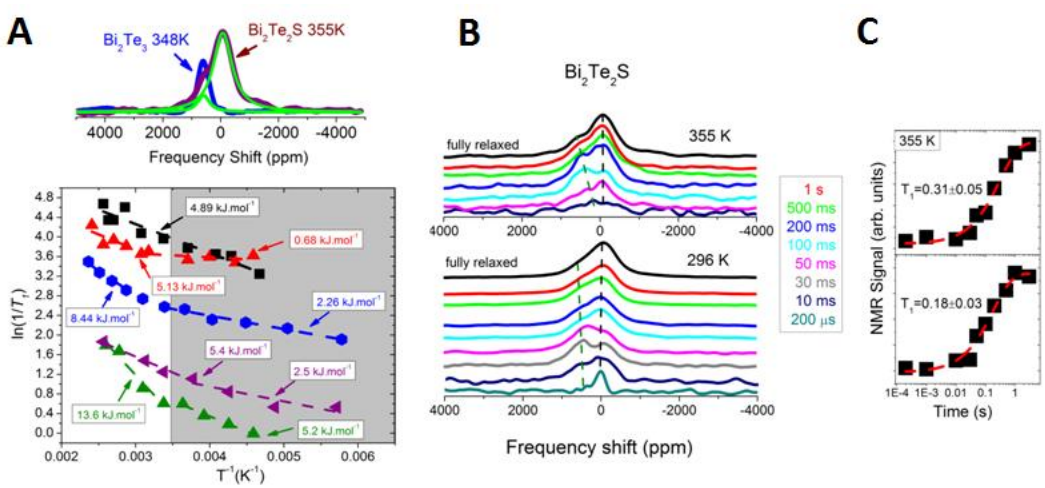

Figure 1. The ^{125}Te NMR spectra for the phase separated Bi_2Te_2S (purple line) at 355 K and Bi_2Te_3 (blue line) at 348 K. The shoulder peak at more positive shifts of Bi_2Te_2S corresponds to the

S-poor Bi_2Te_3 phase which is in agreement with the powder X-ray diffraction pattern analysis. The natural logarithm of the ^{125}Te spin-lattice relaxation rate in the case of $Bi_{0.5}Sb_{1.5}Te_3$ (■), Sb_2Te_3 (▲), Bi_2Te_3 (⬢), Bi_2Te_2S (◀) and Bi_2Te_2S (◆) as a function of the inverse temperature (A). Below 270 K, a second mechanism dominates the spin-lattice relaxation. Comparison of the ^{125}Te spectrum for the phase-separated Bi_2Te_2S at 355 K and 296 K obtained in the saturation recovery experiment after saturation of 200 μs to 3 s (B). Relaxation recovery is not uniform across the resonance. The red line are fitted to a stretched exponential saturation-recovery model with the β=0.7 (C).

To date, electrical transport measurements, scanning tunneling microscopy (STM) and angle resolved photoemission spectroscopy (ARPES) have been the main workhorses for the study of surface states of chalcogenides. These techniques work best at low temperatures (<30 K) with high-quality thin films (<20 nm) or large single crystals . There is, however, a need for characterizing materials at room temperature or materials of suboptimal quality. To this end, magnetic resonance methods are non-invasive local probes of magnetism and the electronic wavefunction in narrow- (and wide)-gap semiconductors. It has been used to study the bulk semiconductor properties of various chalcogenides[7-11], as well as the properties of TI nanoparticles[13,21] and thin films[12]. Worthwhile aspects of the NMR readout include: (i) potential operation at higher temperatures and ambient conditions, (ii) ability to probe lower quality or amorphous materials, (iii) study of “granular” varieties, and (iv) materials with a large number of bulk defects with topologically protected gapless modes. Consequently, magnetic resonance techniques could serve as a complementary tool to characterize materials which are not suitable for study by conventional methods (transport, ARPES, STM). Of great interest is the development of local probes of the material’s bulk region, which is difficult to interrogate independently from the surface states. Two of my previous research investigations on comparative studies of the bulk (and surface) states of multiple TI[9,10] and topological crystalline insulators (TCI)[11] materials relate the NMR results to existing transport and ARPES studies and straightforwardly confirmed that the undesired presence of defects in the bulk state not only affect the TI surface properties[12,13,21] but also can be directly reflected in the NMR parameters (Fig.1).

Lastly, NMR provided the first experimental evidence about the existence of phase separation in TI materials, such as in the Bi_2Te_2S composition[9]. Due to the high sensitivity of the NMR technique to sample defects[9], homogeneity and carrier concentration[7,8], my studies elucidated that the ordered ternary compound Bi_2Te_2Se is the best TI material among the known TIs. This is due to the bulk state remaining insulating across the entire temperature range, allowing the surface states to dominate the material’s conductivity[9,10].

All these aforementioned studies yield non-invasively a local picture of the TI profile (electronic and structural properties). Charge carriers, defects, vacancies and transition metal-ion dopants were explored in relation to the spin degrees of freedom (electronic and nuclear). A characteristic example was my paper which is the first to have detected metallic surface states in TIs in solid-state NMR experiments[12,13]. As shown in Fig. 2, ^{125}Te (Fig. 2A) and $^{121/123}$Sb (Fig. 2B) NMR results on Sb_2Te_3, $Bi_{0.5}Sb_{1.5}Te_3$ and Bi_2Te_3 nanocrystals as functions of particle size and temperature revealed that the nuclear spin-lattice relaxation is enhancedfo particle sizes below 33 nm and is accompanied by a transition of the NMR spectra from a single resonance to a bimodal regime. The satellite peak features a negative Knight shift and higher relaxivity, accompanied with a Korringa law in the range 140-420 K; whereas micrometer particles do so only below 200 K. Comparisons of NMR shift and relaxation rates for various binary TI and non-TI materials (ZnTe, PbTe, PbSe etc.) were performed as control experiments. The results clearly reveal increased metallicity of the nanoscale TIs in the limit of higher surface-to-volume ratios. Additionally, by using the radioactive ion beam spin resonance experiments at TRIUMF we provided (in collaboration with TRIUMF) nanoscale magnetic resonance images through the depth of the material, enabling us to visualize electronic and magnetic properties at edges or interfaces. These striking results demonstrate, for the first time, NMR detection of the TI properties at the nanoscale. Additional studies from magnetically doped TI heterostructures demonstrated our ability to differentiate a topological insulator and magnetic TI layers within the bulk or at the surface of the TI (Fig.2C). These measurements do not require the use of ionizing radiation or a flow of electrons.

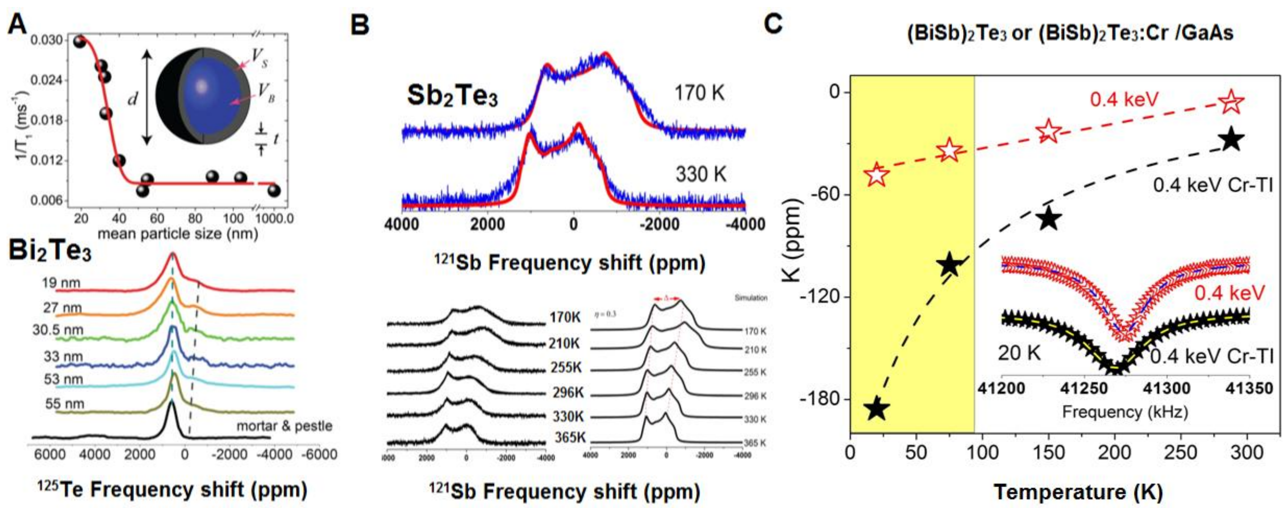

Figure 2. ^{125}Te (A) and ^{121,123}Sb NMR (B) experimental spectra and relaxation rates data of Bi_2Te_3 and Sb_2Te_3 nanocrystals accompanied with the simulated spectra. *β*-NMR spectra and Knight shift of TI and magnetically doped TI (0.4 keV) versus temperature and implantation energies (C).

These studies gave us precise, non-invasive measurements of material properties such as hyperfine coupling constants, relaxation rates ($1/T_1$, $1/T_2$), carrier density, spin-orbit coupling strength as well as the temperature and doping impact on the TI efficiency (Fig. 1,2). In other words, we now have an entirely new set of metrics by which the bulk and surface properties of a TI can be examined. For example, in bulk semiconductors NMR can reveal multiple carrier fractions corresponding to different *n*- or *p*-type fractions whereas transport measurements reveal only a single (averaged) component[7,8].

II. Exploring the rich phase diagrams of the Mott & Topological Insulators for the development of novel energy conversion devices & Superhard Applications (Theory and Experiment)

Electron- or hole-doped transition metal oxides are famous for their extraordinary charge transport properties, including high temperature superconductivity (cuprates) and colossal magnetoresistance (manganites). Astonishingly, the mother system of these compounds is a Mott insulator[1], in which the establishment of the metallic or superconducting state arises from the way that the holes are self-organized with doping. The physics underlying the complex phenomena in these doped perovskites still remains shadowy[1]. In the case of $La_{1-x}Ca_xMnO_3$ (LCMO), competition among different interactions in these systems generates spectacular phenomena, such as the formation of charge and spin textures associated with a commensurate or an incommensurate (IC) modulation, mesoscopic phase separation, and the colossal magnetoresistance (CMR) effect[22]. At the same time frustration of interactions gives rise to the appearance of freezing and glassiness at the lowest and the highest temperatures of the phase diagram, respectively[23]. The appearance of these complex properties is associated with characteristic NMR phenomena like the wipe-out effect and structural or magnetically distorted NMR lineprofiles, expressed with slow relaxation, aging, and other signatures of strongly correlated systems.

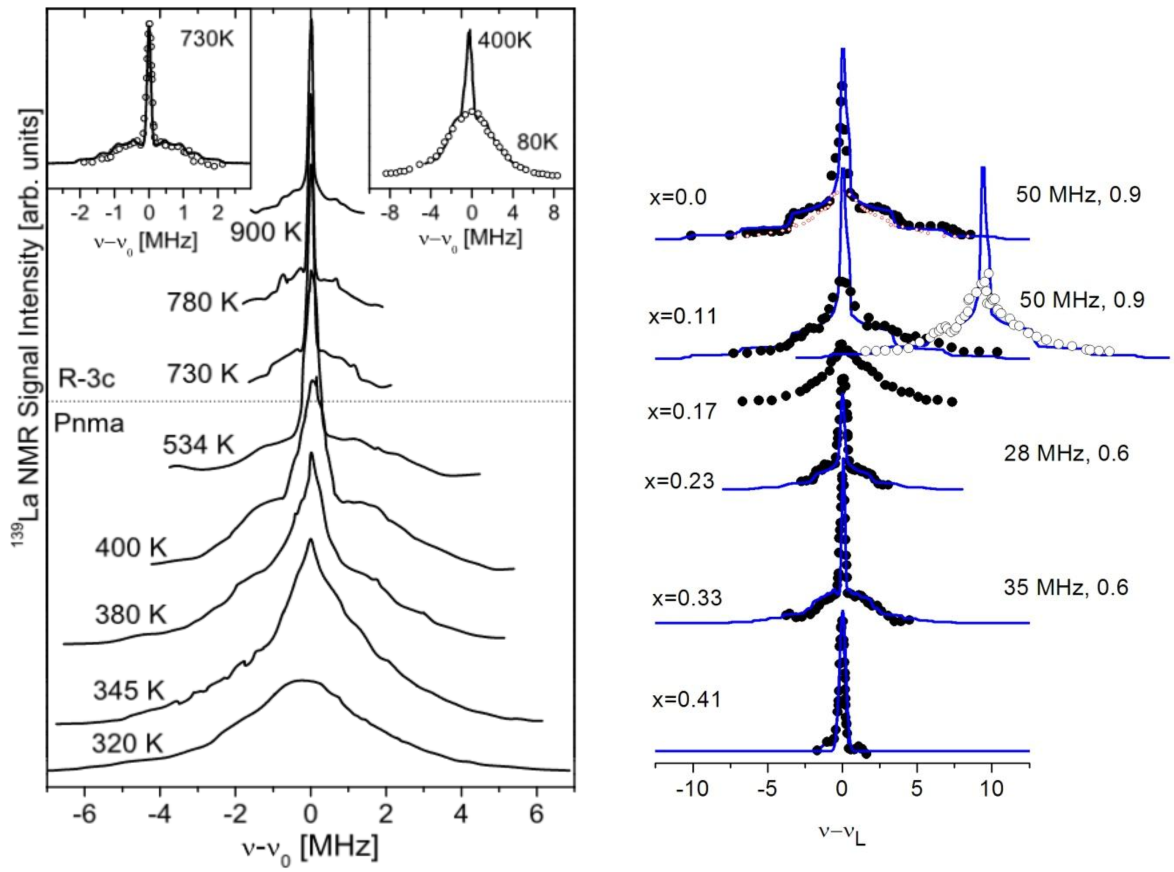

Figure 3. ^{139}La NMR spectra for optimally doped LCMO(0.33), in 9.4 Tesla external magnetic field, as a function of temperature. Spectra are presented relatively to the central line frequency ν_0. The dotted line shows schematically the border line between the *R-3c* and *Pnma* phase regimes. The left inset depicts the calculated powder pattern spectrum in comparison to the experimental spectrum at T = 730K (left panel). The right inset shows a comparison of spectra at 80K (open circles) and 400K (solid line). ^{139}La NMR spectra for LCMO x = 0.11,0.17,0.23,0.33,and0.41 at 500K, in 9.4 Tesla external magnetic field. Spectra are presented relatively to the central line frequency ν_0. Open circles are experimental data and solid lines theoretical simulations. The inset indicates the electric quadrupolar coupling as a function of doping (right panel).

NMR may be uniquely used as a probe of intricate magnetic and structural features in ferromagnetic and antiferromagnetic colossal magnetoresistive manganites. On the basis of my previous experimental results I have demonstrated that the undoped compound ($LaMnO_3$), which is an antiferromagnetic insulating compound, shows a unique NMR profile accompanied with the powder pattern which reflects the predominant quadrupolar character of this compound[22]. With the addition of holes, the homogeneous antiferromagnetic insulating phase transforms to an inhomogeneous ferromagnetic metallic phase ($0.2<x<0.45$) which is expressed by a magnetic broadening of the NMR lineprofiles and alteration of the spin-relaxation rates[23]. Specifically, at the higher temperatures in which the system is a paramagnet, the structural transformation from orthorombic to rhombohedral is associated with the narrowing of the NMR lineprofiles and the appearance of the satelite frequency distributions (Fig. 3)[22,23]. Different calcium dopings induce changes in the satelite distribution. This reflects the local lattice distortions produced a spin glass state. In the case of overdoped manganites (x>0.5), the NMR measurements provided evidence that the ground state in overdoped LCMO manganites comprises an IC soliton-modulated spin density wave[24]. At higher temperatures the modulation wave transforms to a uniform IC plane wave, which is subjected to strong slow fluctuations, as implied by the complete wipeout effect[23,24] of the NMR signal. On the one hand by lowering temperature I have shown that the narrow NMR spectra observed in the antiferromagnetic (AFM) phase are shown to wipe out, while for $T < 30K$ a very broad spectrum reappears, characteristic of an IC charge and spin modulation. Remarkably, by further decreasing temperature, a relatively narrow feature emerges from the broad IC NMR signal, manifesting the appearance of a solitonic modulation as $T \rightarrow 0$ (Fig. 4). On the other hand, by increasing the temperature up to 1000 K, I have shown for the first time the presence of magnetic polarons in the paramagnetic (PM) regime of underdoped LCMO and other high-Tc superconductors[22,24]. This research study provided the first direct evidence that the spin ground state in overdoped manganites is solitonic instead of charge stripes and has attracted considerable media interest[25] that appeared with the title " *Research findings from D. Koumoulis et al update understanding of physics*".

More recently, X-ray diffraction and neutron scattering studies in heavily doped manganites revealed the formation of superstructures associated with the presence of magnetic and structural superlattice Bragg peaks. Correlation between similar superlattices and "exotic" ordered phases has been found in other complex oxides such as cuprates and nickelates. However, recent experiments in overdoped manganites of the $La_{1-x}Ca_xMnO_3$ (LCMO) family have shown that instead of charge stripes, charge in these systems is organized in a uniform charge density wave (CDW). Therefore, understanding these intrinsic electronic heterogeneities of Mott insulators still remains an arguable field in the study of unconventionally condensed matter physics phenomena.

A static and dynamic investigation of magnetic states by NMR should be a powerful probe for the unexplored heavily doped regime of Mott insulators. In ^{139}La and ^{55}Mn NMR the lanthanum and manganese nuclei directly exhibit the magnetic state (FM or AF) of the nearest oxygen and manganese ions neighbors. ^{139}La, ^{55}Mn and ^{17}O NMR should reveal the nature of the ground state of cuprates and pnictides and provide evidence if it is topologically trivial or topologically protected[24]. These classes of materials also show improved mechanical properties and advancing photovoltaic efficiency[27].

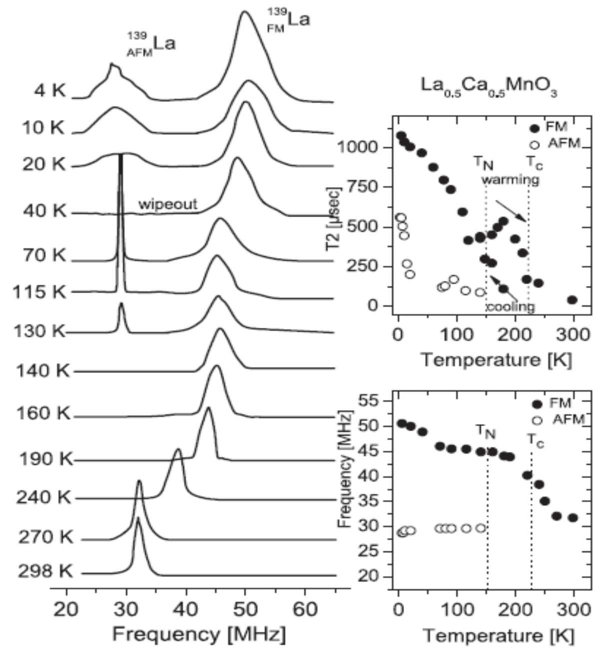

Figure 4. [139]La NMR spectra for LCMO 0.50 at various temperatures. The upper right hand panel shows the spin-spin relaxation time T_2 vs T for both the FM and AFM signal components. The lower right-hand panel shows the corresponding signal frequencies.

Outreach Goals and Objectives

The goal of my research projects is to investigate and vastly enlarge the number and type of existing Topological and Mott insulating materials in order to understand the nature of TI and Mott properties as well as their thermoelectric, spintronic and mechanical (hardness) properties in strongly correlated systems. The overall experience that I have accomplished during my PhD research and postdoctoral appointment on TIs and the strongly correlated electron systems has now been translated into "know-how" for detecting their exotic physical properties. The introduction of strongly correlated electron modes in TEs and TIs will fundamentally alter the properties of the topological phases in ways that could improve the material properties while giving rise to exotic new physics through the design of phase-separated materials such as manganites, hexaborides, transition metal borides etc. The combination of Mott and Topological insulators could help us understand the exotic nature of the surface states, probe their properties in proximity to other materials and lead to systems that exhibit better insulating bulk and ultra robust surface states. Also, there are plenty of unexplored areas in these materials that I would also like to study. One of the most interesting is the investigation via high-temperature NMR study of the *Emphanisis*[29] in SnTe, PbS and PbTe, a locally distorted high-temperature state, which emerges on warming from an undistorted rock salt structure. In a previous variable temperature NMR study[11], I have shown that the band-gap evolution of Pb-based chalcogenides is non-trivial due to the band inversion phenomenon[11]. I would like to investigate this unconventional band-gap evolution in

$Pb_{1-x}Sn_xTe$ as function of pressure via high-pressure assisted NMR studies. In conclusion, what is the underlying mechanism that governs the relative energies as a function of temperature for two valence bands (L and Σ)[30] in the lead based chalcogenide systems? All these marvelous subjects in semiconductor physics remain under debate and would be part of my research endeavors. Accordingly, this research project will bring new experimental tools that could have applications to nanotechnology in the search for dissipationless devices, optoelectronics, spin-orbitronics, mechanical and anticorrosive applications[26] and optimized current thermoelectric generators[3,4]. I will maintain my current collaborations and by creating new ones I can guarantee the access to facilities with state-of-the-art capabilities and a well-established interdisciplinary research in the area of Inorganic/Materials Chemistry.

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