JANUARY 23–24, 2017

Strongly Correlated Materials

TOPOLOGY AND QUANTUM PHASE TRANSITIONS
# Table of Contents

- Presentation Guidance ............................................................................................................... 1
- Agenda ........................................................................................................................................ 2
- Invited Speakers ....................................................................................................................... 5
- About RCQM ............................................................................................................................. 6
- RCQM Membership .................................................................................................................. 7
- RCQM Advisory Board ............................................................................................................. 8
- Speakers ..................................................................................................................................... 9
- Poster Presentations ................................................................................................................... 26
- Rice University Campus Map .................................................................................................... 32
Rationale and Scope

Topological states of matter are actively being explored in strongly correlated electron materials. Because strong correlations lead to a host of electronic ground states, this subject is inherently entwined with the physics of quantum phase transitions.

The workshop will address open questions and explore new directions in the areas of topology and quantum phase transitions in Kondo insulators, heavy fermion metals, and related materials. It will bring together experts in these different focus areas so that lively discussions can take place.

Oral sessions

All oral sessions will be held in McNair Hall, Room 116.

Poster Session

The poster session will be held in the Rice University Student Center, Grand Hall.

WIRELESS INTERNET ACCESS

Wireless access is available through the wireless network ‘Rice Visitor.’ Simply select this network, agree to the terms and conditions, and you should have full access, including electronic journals supported by the Rice library.
Welcome Remarks
8:40 am Douglas Natelson
Chair, Department of Physics and Astronomy, Rice University

Session 1 — Topology and Correlations: Experimental Perspective
Chair: Joe D. Thompson (Los Alamos National Laboratory)

8:45 – 9:15 am Silke Bühler-Paschen (Vienna University of Technology/Rice University)
Topology and Quantum Phase Transitions in Heavy Fermion Materials

9:15 – 9:45 am Zachary Fisk (University of California, Irvine)
Comparison of Kondo Insulating Properties of SmB\(_6\) and YbB\(_6\)

Session 2 — Topology and Correlations: Theoretical Perspective
Chair: Joe D. Thompson (Los Alamos National Laboratory)

9:45 – 10:15 am Pavan Hosur (University of Houston)
Time-reversal Invariant Topological Superconductivity in Doped Weyl Semimetals

10:15 – 10:45 am Break

10:45 – 11:15 Qimiao Si (Rice University)
Strong Correlations and Spin-Orbit Couplings in Kondo Lattice Systems

11:15 – Noon Discussion

Lunch
Rice University Student Center, Grand Hall
Noon – 1:30 pm

Session 3 — Kondo Insulators and Related Materials
Chair: Matthew Foster (Rice University)

1:30 – 2:00 pm Johnpierre Paglione (University of Maryland)
Surface Ferromagnetism and 1D Edge State Transport in SmB\(_6\)

2:00 – 2:30 pm Suchitra Sebastian (University of Cambridge)
Identifying Exotic Electronic Ground States Using Quantum Oscillations: The Case of the Kondo Insulator SmB\(_6\)
Session 4 — Theory of Topology and Quantum Phase Transitions
Chair: Pengcheng Dai (Rice University)

Tuesday, January 24, 2016
McNair Hall, Room 116

8:45 – 9:15 am  Maxim Dzsero (Kent State University)
Unconventional Physics of Conventional Kondo Insulators

9:15 – 9:45 am  Fakher Assaad (University of Wuerzburg)
A Study of Topology and Quantum Phase Transitions from Monte Carlo Simulations

9:45 – 10:15 am  Andriy Nevidomskyy (Rice University)
Topological Nodal Superconductivity, Surface States and the Role of Disorder in UPt$_3$

10:15 – 10:45 am  Break

10:45 – 11:15 am  Catherine Pépin (CEA, France)
Emergence of Superconductivity in the Presence of Two Kinds of Fluctuations

11:15 am – Noon  Discussion

Noon – 12:15 pm  Poster Preview Session
Workshop on Strongly Correlated Materials

Lunch and Poster Session
Rice University Student Center, Grand Hall
12:15 pm – 2:30 pm

Session 5 — Emergent Phases and Quantum Criticality
Chair: Meigan Aronson (Texas A&M)

2:30 – 3:00 pm  Collin Broholm (Johns Hopkins University)
*Incommensurate Magnetism in Ce-based Heavy Fermion Systems*

3:00 – 3:30 pm  Yuji Matsuda (Kyoto University)
*Emergent Exotic Superconductivity in Artifically Engineered Kondo Superlattices*

3:30 – 4:00 pm  Joe D. Thompson (Los Alamos National Laboratory)
*Pressure-Induced Quantum-Phase Transitions in a Heavy-Fermion Metal*

4:00 – 5:00 pm  Discussion
<table>
<thead>
<tr>
<th>Invited Speakers</th>
<th>Institution</th>
</tr>
</thead>
<tbody>
<tr>
<td>James Analytis</td>
<td>University of California, Berkeley</td>
</tr>
<tr>
<td>Fakher Assaad</td>
<td>University of Wuerzburg</td>
</tr>
<tr>
<td>Collin Broholm</td>
<td>Johns Hopkins University</td>
</tr>
<tr>
<td>Silke Bühler-Paschen</td>
<td>Vienna University of Technology/Rice University</td>
</tr>
<tr>
<td>Jonathan Denlinger</td>
<td>Lawrence Berkeley National Lab</td>
</tr>
<tr>
<td>Maxim Dzsero</td>
<td>Kent State University</td>
</tr>
<tr>
<td>Zachary Fisk</td>
<td>University of California, Irvine</td>
</tr>
<tr>
<td>Pallab Goswami</td>
<td>University of Maryland</td>
</tr>
<tr>
<td>Pavan Hosur</td>
<td>University of Houston</td>
</tr>
<tr>
<td>Yuji Matsuda</td>
<td>Kyoto University</td>
</tr>
<tr>
<td>Andriy Nevidomskyy</td>
<td>Rice University</td>
</tr>
<tr>
<td>Johnpierre Paglione</td>
<td>University of Maryland</td>
</tr>
<tr>
<td>Catherine Pépin</td>
<td>CEA, France</td>
</tr>
<tr>
<td>Suchitra Sebastian</td>
<td>University of Cambridge</td>
</tr>
<tr>
<td>Qimiao Si</td>
<td>Rice University</td>
</tr>
<tr>
<td>Lucia Steinke</td>
<td>Texas A&amp;M University</td>
</tr>
<tr>
<td>Joe D. Thompson</td>
<td>Los Alamos National Laboratory</td>
</tr>
</tbody>
</table>
About RCQM

Mission Statement

Rice University’s Center for Quantum Materials seeks to sustain and grow fundamental research of quantum materials on campus, and develop an international network in this area, with Rice at its hub. The center will incubate new research collaborations and directions by organizing scientific workshops, supporting distinguished visitors to Rice, sponsoring postdoctoral scholars and student researchers and developing international and domestic partnerships.

From left: Ned Thomas, dean of the George R. Brown School of Engineering; Yousif Shamoo, Vice Provost for Research; Peter Rossky, dean of the Wiess School of Natural Sciences; Qimiao Si, director of the Center for Quantum Materials; Pulickel Ajayan, the Benjamin M. and Mary Greenwood Anderson Professor in Materials Science and NanoEngineering and of chemistry; and Tom Killian, department chair and professor of physics and astronomy.
RCQM Membership

**ATOMIC, MOLECULAR AND OPTICAL ENGINEERING**
- Kaden Hazard
- Randy Hulet *
- Tom Killian
- Han Pu

**CONDENSED MATTER**
- Pengcheng Dai *
- Rui-Rui Du
- Matthew Foster
- Emilia Morosan

- Doug Natelson
- Andriy Nevidomskyy
- Qimiao Si * Director

**ELECTRICAL AND COMPUTER ENGINEERING**
- Palash Bharadwaj
- Kevin Kelly
- Jun Kono *
- Gururaj Naik
- Isabell Thomann

**MATERIALS SCIENCE AND NANOENGINEERING**
- Pulickel Ajayan
- Jun Lou
- Emilie Ringe
- Boris Yakobson *

**CHEMISTRY**
- Peter Rossky
- Gus Scuseria
- James Tour

*Executive Committee Members*
Thanks and Appreciation

RCQM would like to express our appreciation to the members of the Advisory Board for their continued time and dedication to the center.

Frank Steglich
Max Planck Institute for Chemical Physics of Solids, Dresden

Hongjie Dai
Stanford University

Laura Greene
University of Illinois at Champaign-Urbana

Meigan Aronson
Texas A&M University

Allan H. MacDonald
University of Texas at Austin

Jason Ho
Ohio State University

Elihu Abrahams
UCLA
(not pictured)
Weyl Wiggles: Exotic Quantum Oscillatory Phenomena in Weyl and Dirac Semi-metals

Dirac semi-metals show a linear electronic dispersion in three dimensions described by two copies of the Weyl equation, a theoretical description of massless relativistic fermions. At the surface of a crystal, the breakdown of fermion chirality is expected to produce topological surface states without any counterparts in high-energy physics nor conventional condensed matter systems, the so-called “Fermi Arcs”. Here we present Shubnikov-de Haas oscillations in Focused Ion Beam prepared microstructures of Cd3As2 that share characteristics of surface and bulk states as expected for “Weyl orbits”, the theoretically predicted cyclotron path that weaves together Fermi arc and chiral bulk states. In contrast to conventional cyclotron orbits, these are governed by the chiral bulk dynamics rather than the common momentum transfer due to the Lorentz force. Our observations provide evidence for direct access to the topological properties of charge in a transport experiment, a first step towards their potential application.

James Analytis joined the faculty at UC Berkeley in January 2013 as the Charles Kittel Chair in condensed matter physics. He received his B.Sc. in physics from Canterbury University in 2001 and his D. Phil. from the University of Oxford as a Rhodes’ Scholar in 2006. At Oxford, he worked with Stephen Blundell and Arzhang Ardavan on experimental and computational studies of quasi-two dimensional organic superconductors. Following his graduate studies, Analytis was a Lloyd’s Tercentenary Fellow at the University of Bristol, where he worked on understanding the nature of anisotropic scattering in cuprate superconductors. In 2008 he became a post-doctoral fellow at Stanford University where he worked on both pnictide superconductors and topological insulators. In 2010 Analytis became a staff scientist at the Stanford Institute for Materials and Energy Science. The Analytis lab at Berkeley is capable of creating new materials and characterizing their thermodynamic and transport properties, particularly in the presence of high magnetic fields.
A Study of Topology and Quantum Phase Transitions from Monte Carlo Simulations

In this talk I will review recent progress in quantum Monte Carlo simulations of correlated electron systems. This progress allows the study of a variety of phenomena including de-confined phases and phase transitions, instabilities of Dirac metals as well as the competition of classical frustration and Kondo screening.
Incommensurate Magnetism in Ce-based Heavy Fermion Systems*

I shall discuss neutron scattering experiments probing incommensurate magnetism in cerium based heavy fermion systems including CeNiAsO, CeAuSb$_2$, and CeCoGe$_3$. While local moment concepts such as crystal field effects and competing RKKY interactions are helpful to correlate magnetic measurements, the transport anomalies and magnetic field effects in these materials call for an itinerant approach and challenge our understanding of strongly correlated 4f-electrons.

*Guy Marcus, Chris Stock, and Shan Wu, were major contributors to this work. IQM is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Material Sciences and Engineering under Grant No. DE-FG02-08ER46544.
Silke Bühler-Paschen, Ph.D.

Topology and Quantum Phase Transitions in Heavy Fermion Materials

The excellent tunability of heavy fermion metals by non-thermal control parameters such as magnetic field, pressure, or doping has vastly expanded our understanding of these materials. In particular it has brought to light quantum criticality at the border of different ordered phases, Landau and beyond Landau quantum criticality, as well as “naked” quantum critical points (QCPs) and QCPs covered by domes of new phases [1]. By comparison, the larger energy scales governing Kondo insulators, their (pseudo)gapped sister compounds, has severely limited similar studies in this class of materials [1]. The recent discovery that a new tuning parameter, spin-orbit coupling, can be realized in certain substitution studies and leads to a crossover between a Kondo insulator and semimetal [2] with characteristics of a recently proposed Weyl-Kondo semimetal [3] may bring new impetus to the field.

We acknowledge financial support from the Austrian Science Fund (projects I2535-N27 and W1243-N16) and the ARO grant W911NF-14-1-0496.

References:

Silke Bühler-Paschen is an experimental condensed matter physicist, working in the fields of strongly correlated electron systems and thermoelectrics. She graduated in physics from Graz University of Technology in Austria, with an external diploma work at the Paul Scherrer Institute in Switzerland. After her PhD studies at EPFL in Lausanne and a postdoctoral stay at ETH Zurich she moved to Germany, where she joined the Max Planck Institute for Chemical Physics of Solids in Dresden, first as scientific collaborator and then as associate professor. After a visiting professorship at the Nagoya University in Japan she was appointed full professor at the Vienna University of Technology in Austria. She received a C3 professorship from the Excellence Program of the Max Planck Society for the Advancement of Outstanding Female Scientist in 2003 and an ERC Advanced Grant from the European Research Council in 2008. She is APS fellow and leader of various national and international research projects. Her team is active in materials synthesis and characterization, using a large pool of different physical property measurements under multiple extreme conditions — spanning, for instance, 7 orders of magnitude in temperature. Topics of current interest include quantum criticality, heavy fermion systems, Kondo insulators, new topological phases, and thermoelectrics.
Outstanding Issues for the Topological Scenario of SmB$_6$

The mixed valent compound SmB$_6$ was the first candidate example of a new class of strongly correlated topological insulators, with the new TI surface state scenario providing an elegant explanation for a long time mystery of residual conductivity <4K in the insulating phase. Similar to other TI materials, the physical realization of the TI surface properties in surface-sensitive angle resolved photoemission (ARPES) measurements must compete with other possible non-topological materials issues including surface relaxation, surface reconstruction, (001) polar surface termination(s) and surface band bending, and weaker f-d hybridization at the surface (e.g. surface Kondo breakdown). An assessment of these various effects as viewed by ARPES is reviewed for SmB$_6$ in comparison to other non-topological divalent [1] and trivalent hexaborides including both (001) and (110) cleaved and prepared surfaces.

In addition from this renewed interest in SmB$_6$, temperature-dependent ARPES and dynamical mean field theory (DMFT) calculations have provided new insights into the evolution of the bulk mixed-valent 4f electronic structure and hybridization gap formation [2]. In particular, an important role of f-p hybridization is identified in the formation of the insulating gap, which goes beyond the minimal two-band models of f-d hybridization. In addition a dimensional crossover evolution 3D bulk d-band states crossing $E_F$ to 2D helical in-gap surface states is observed to be intimately linked to the bulk gap evolution.

References:

Dr. Jonathan Denlinger works in experimental condensed matter physics, with an emphasis on synchrotron-based angle-resolved photoemission of f-electron and strongly correlated electron systems. Dr. Denlinger obtained his B.S. degree in Physics from Purdue University, and his Ph.D. degree in Physics from the University of California, Berkeley in 1993. He did his postdoctoral works at the Advanced Light Source, commissioning a photoemission beamline in collaboration with U. of Wisconsin-Milwaukee, and at the University of Michigan where he was introduced to f-electron physics. In 1999 he joined the staff at the ALS as a beamline scientist first for a beamline specializing in x-ray absorption and emission and then at a newer high-resolution ARPES beamline.
Unconventional Physics of Conventional Kondo Insulators

The physics of samarium hexaboride — a narrow gap strongly correlated semiconductor discovered almost 50 years ago — continues to inspire experimental and theoretical research. Much of the recent work has been motivated by theoretical proposals that samarium hexaboride provides a prototypical example for the first correlated $Z_2$ topological Kondo insulator. In this talk I will first outline the main ideas, which lead to realization that samarium hexaboride becomes a topological Kondo insulator below a certain temperature. Then, I will discuss recent theoretical works, which address several experiments, which should help to identify the topological nature of the metallic surface states. Finally, I will review recent experimental works which challenge our current understanding of physics of this fascinating material.
Comparison of Kondo Insulating Properties of SmB$_6$ and YbB$_6$

The high pressure studies of Sun$^1$ provide evidence the YbB$_6$ becomes a topological insulator in the vicinity of 20GPa. We review this evidence and the questions that the data raises concerning the fundamental differences between ordinary divalent hexaborides and SmB$_6$ and YbB$_6$.

Fisk received his PhD from UC San Diego in 1969 as a student in the group of B.T.Matthias. He subsequently held positions at the University of Chicago, UC San Diego, Los Alamos National Laboratory, Florida State University and UC Davis prior to his present position at UC Irvine. His primary interests are in superconductivity and heavy Fermion materials.
Signatures of Topological Weyl Semimetal in Correlated Materials

The Weyl fermions can describe low energy quasiparticles of inversion or time reversal symmetry breaking states in three dimensional materials [1]. They combine seemingly disjoint notions of critical bulk excitations and nontrivial momentum space topology, and support many exotic bulk transport and electrodynamic properties in addition to protected, zero-energy surface states (Fermi arcs). In weakly correlated materials, the angle resolved photoemission spectroscopy provides strong evidence for coherent Weyl fermions in the bulk and Fermi arcs on the surface. However, their spectroscopic detection in a correlated material can be complicated by interaction induced short life time and bandwidth suppression, thus requiring complementary measurements of transport and electrodynamic properties, which are sensitive to the underlying topology. I will discuss such signatures of Weyl fermions, including the large anomalous Hall conductivity [2], the optical activity [3], and the chiral anomaly induced negative longitudinal magnetoresistance [4]. I will argue that combined spectroscopic and transport measurements can unveil elusive Weyl excitations in many correlated materials.

References:

Pallab Goswami is currently a postdoctoral fellow at Condensed Matter Theory Center, University of Maryland. He is interested in developing new theoretical tools for addressing emergent quantum phases and phase transitions in strongly correlated and disordered materials, with an emphasis on topological properties. He received his PhD in 2008 from University of California, Los Angeles. Subsequently, he has carried out postdoctoral research at Rice University, National High Magnetic Field Laboratory at Tallahassee, before moving to University of Maryland in 2014.
Time-reversal Invariant Topological Superconductivity in Doped Weyl Semimetals

High-school physics categorizes matter into solids, liquids and gases, based on its ability to fill up a given container. By the end of an undergraduate course in solid state physics, one learns that matter can also be classified based on its ability to transport charge, as a metal, insulator, semiconductor or a semimetal. Finally, a graduate course in condensed matter physics informs us of the traditional classification of states of matter – the Landau theory – based on which symmetry the ground state breaks that the Hamiltonian does not. However, the last three decades have shown us that even this picture is incomplete – matter can be characterized by topological properties of the ground state wavefunction in addition to its broken symmetries.

This talk will introduce the basic ideas behind how topological labels can be applied to electronic band structures, and focus on a phase that has gained tremendous attention in the last few years, namely, Weyl semimetals. It will be highlighted that doped Weyl semimetals form a natural platform for another topological state of matter, viz., a time-reversal invariant topological superconductor in three dimensions. The latter has no known realizations in electronic systems thus far. Finally, it will be shown, within a fluctuation-exchange approach, that doped Na3Bi with broken inversion symmetry and ferromagnetic interactions has an instability towards such a superconductor.

Prof. Pavan Hosur’s research interests are in theoretical condensed matter physics and quantum statistical mechanics. Within condensed matter theory, he is currently excited about topological phases of matter, especially gapless ones such as Dirac and Weyl semimetals. He is also interested in exploring unusual broken symmetry phases and devising ways to detect them in experiments. Questions in quantum statistical mechanics that he is thinking about revolve around quantum ergodicity, quantum chaos, and generally, how ideas from classical statistical mechanics apply to quantum systems. These questions have received a surge of interest lately via work on Eigenstate Thermalization and Many-Body Localization, but many aspects remain unclear. Hosur hopes to understand and contribute toward resolving them in the coming years.
Emergent Exotic Superconductivity in Artifically Engineered Kondo Superlattices

In the presence of inversion symmetry breaking, strong spin-orbit coupling dramatically affects the superconductivity through the Rashba splitting. It has been proposed that cooperative effect of electron correlations and Rashba splitting provide notable effects on superconductivity, leading to exotic superconducting states such as helical or stripe phases, but such phases have never been reported so far. We have fabricated Kondo superlattices consisting of alternating layers of YbCoIn$_5$, CeCoIn$_5$ and YbRhIn$_5$ with atomic thicknesses, where CeCoIn$_5$ is a $d$-wave superconductor and YbCoIn$_5$ and YbRhIn$_5$ are conventional metals. In these “tricolor” superlattices where the magnitude of the Rashba splitting can be tuned, in-plane upper critical field $H_{c2}$ exhibits an anomalous upturn at low temperatures, indicating a possible emergence of helical or stripe superconducting phase.

We also fabricate CeCoIn$_5$/CeRhIn$_5$ superlattices, where CeRhIn$_5$ is a heavy fermion SDW compound. In these “hybrid” superlattices, $d$-wave superconductivity coexists with SDW at ambient pressure. Under high pressure with approaching SDW QCP of CeRhIn$_5$ layers, $H_{c2}/T_c$ is strikingly enhanced, suggesting an emergence of extremely strong coupling superconductivity.

Yuji Matsuda received his Ph.D. in Physics from the University of Tokyo (Japan) in 1987 and became a research associate at Department of Pure and Applied Science, the University of Tokyo. He became an associate professor in 1993 at Hokkaido University (Japan) after spending two years at Princeton University (USA) as a postdoctoral fellow. He moved to Institute for Solid State Physics, University of Tokyo, as an associate professor in 1997, and became a full professor at Kyoto University in 2004. He is a condensed matter experimentalist with interests in electronic and magnetic properties of solids. His current research interests include strongly correlated electron systems, in particular exotic superconductivity, heavy fermion systems, high-$T_c$ superconductors, and quantum spin systems.
Topological Nodal Superconductivity, Surface States and the Role of Disorder in UPt$_3$

The concept of topological states of matter has captured the imagination of physicists in the last decade. Traditionally, such topological phases are predicted to occur in fully gapped insulating or superconducting materials and are characterized by topologically protected gapless excitations on the surface [1]. Here, I will demonstrate a generalization of this concept to metallic materials with gapless bulk excitations, focusing in particular on the B-phase of the heavy fermion superconductor UPt$_3$. Phase sensitive measurements provide strong evidence for the triplet, chiral pairing symmetry in UPt$_3$, which endow the Cooper pairs with orbital angular momentum $L_z = \pm 2$ along the $c$-axis [2]. Such pairing supports both line and point nodes of the superconducting gap, and I show that both types of nodal quasiparticles possess nontrivial topology in the momentum space. In particular, the point nodes located at the intersections of the closed Fermi surfaces with the $c$-axis act as the double monopoles and the anti-monopoles of the Berry curvature [3]. Consequently, we predict that the B phase should support an anomalous thermal Hall effect, various magneto-electric effects such as the polar Kerr effect, in addition to the topologically protected Majorana arcs on the $(1,0,0)$ and $(0,1,0)$ surfaces [3]. At the transition from the superconducting B-phase to the A-phase of UPt$_3$, the time reversal symmetry is restored, and the topological Andreev surface states disappear. I will also discuss the role of impurities on the topological properties of double-Weyl superconductors and the corresponding Andreev surface states.

References:

Dr. Andriy Nevidomskyy is a theoretical condensed matter physicist, working in the field of strong electron correlations in quantum materials. The collective behaviour of electrons in such materials often results in the emergence of new exotic quantum phases, such as the unconventional superconductivity and quantum spin orders. Nevidomskyy has explored these phenomena in the heavy fermion materials and in the iron-based superconductor. He is particularly interested in the novel quantum phases emerging in frustrated magnets and their topological properties. Originally from Ukraine, he received his PhD in physics from Cambridge University in the UK, before moving to Université de Sherbrooke in Canada as a postdoctoral fellow to work on high-temperature cuprate superconductors. Prior to joining Rice in 2010, he was a postdoctoral researcher in the Center for Materials Theory at Rutgers University, conducting research into heavy fermion materials. He is the recipient of the NSF CAREER Award and the Cottrell Scholar Award from Research Corporation for Science Advancement.
Surface Ferromagnetism and 1D Edge State Transport in SmB$_6$

The Kondo insulator compound SmB$_6$, with hybridization between itinerant conduction electrons and localized f-electrons driving an insulating gap and metallic surface states at low temperatures, is an ideal candidate for realizing the topological Kondo insulator state. I will present our extensive milliKelvin magnetotransport measurements of SmB$_6$ that provide evidence for the existence of surface ferromagnetism. By exploiting the presence of this time reversal symmetry breaking state, we investigate the topological nature of metallic surface states. We find evidence of one-dimensional surface transport with conductance values approaching the quantized value of $e^2/h$ and originating from the chiral edge channels of ferromagnetic domain walls, providing strong evidence that topologically non-trivial surface states exist in SmB$_6$. 
Emergence of Superconductivity in the Presence of Two Kinds of Fluctuations

In this talk we compare the emergence of superconductivity, in the presence of two kinds of fluctuations. First, we explore the vicinity of a magnetic quantum critical point where quantum fluctuations are the pairing glue for the formation of Cooper pairs. In contrast, we present a situation where an emergent symmetry controls the fluctuations in a wide region of the phase diagram, leading to d-wave Cooper pairing in competition with d-wave charge order. Application to high temperature superconductors will be discussed.
Identifying Exotic Electronic Ground States Using Quantum Oscillations: The Case of the Kondo Insulator SmB$_6$

The experimental tool of quantum oscillations have found widespread use in mapping the characteristic electronic structures of strongly correlated materials ranging from heavy fermions to unconventional superconductors. My research focusses on the use of this powerful tool to identify exotic ground states in strongly correlated electron systems. I will present the surprising observation of quantum oscillations from the insulating bulk of the Kondo insulating material samarium hexaboride. An unconventional origin of quantum oscillations is indicated from experimental evidence I will show for novel itinerant low energy excitations. Potential models will be discussed in the context of our findings.

Suchitra Sebastian is Associate Professor in Physics at the University of Cambridge. She searches for exotic quantum phases of matter in new and interesting materials, often by studying them under extreme conditions of high magnetic fields, enormous pressures, and low temperatures. Materials families she studies include unconventional superconductors, and f-electron systems she recently found to display strange dual metal-insulating behaviour.
Strong Correlations and Spin-Orbit Couplings in Kondo Lattice Systems

Strongly correlated electrons represent a vibrant field that continues to expand its horizon. In heavy fermion systems, local moments interact with each other through an RKKY interaction, which contains a variable degree of frustration, and are also coupled to a bath of conduction electrons via the Kondo interaction. Theoretical models of heavy fermion systems consider the interplay between these two types of interactions, which lies at the heart of quantum criticality and a plethora of emergent magnetic and superconducting phases. The underlying physics that goes beyond Landau’s framework is organized by a global phase diagram. There is a rising interest in studying the explicit effect of spin-orbit couplings in such models, and this promises to uncover a new set of phases that are both strongly correlated and topologically non-trivial. An example is the recently predicted Weyl-Kondo semi-metal phase [1], whose key signature has been realized in a new heavy fermion compound [2].

Work supported by the ARO Grant No. W911NF-14-1-0525, and by the NSF Grant No. DMR-1611392 and the Robert A. Welch Foundation Grant No. C-1411.

References:

Prof. Qimiao Si works in theoretical condensed matter physics, with an emphasis on strongly correlated electron systems. One area of Prof. Si’s current interest is quantum criticality. He and his collaborators have advanced a new type of quantum critical point that has considerably shaped the development of the heavy-fermion field. Another focus of Prof. Si’s current research concerns iron-based superconductivity. His work has elucidated the bad-metal behavior in the normal state, and its relationship with magnetism and superconductivity. Prof. Si obtained his B.S. degree in Physics from University of Science and Technology of China in 1986, and his Ph.D. degree in Physics from the University of Chicago in 1991. He did his postdoctoral works at Rutgers University and University of Illinois at Urbana-Champaign. In 1994 he joined the faculty of Rice University, where he is the Harry C. and Olga K. Wiess Professor of Physics. Prof. Si was named a Sloan Research Fellow in 1996, and received a Cottrell Scholar Award from the Research Corporation for Science Advancement in 1998. He was elected a Fellow of the British Institute of Physics in 2004, the American Physical Society in 2005, and the American Association for the Advancement of Science in 2008. He received a Humboldt Prize from the Alexander von Humboldt Foundation in 2012.
Magnetotransport of Surface States in HfNiSn Single Crystals

The large family of half-Heusler compounds hosts a number of topological insulator materials and potential topological superconductors, making these compounds interesting candidates to study physical phenomena on the verge of a topological phase transition. Here we present first magnetotransport measurements on high-quality single crystals of HfNiSn, which according to density functional theory calculations is a nonmagnetic, topologically trivial semiconductor without a bulk band inversion. Our samples show unconventional transport properties already at moderately low temperatures $T < 200$ K. Instead of the thermal carrier freeze-out expected for a bulk semiconductor, electrical conduction in HfNiSn is increasingly dominated by metallic surface states, with a saturation of the longitudinal resistance and highly nonlocal transport. X-ray diffraction shows no structural transitions that could potentially lead to anisotropic conduction in this temperature regime. Magnetoresistance measurements are consistent with weak anti-localization, a signature of low-dimensional transport in a system with strong spin-orbit coupling. The transverse resistance shows an anomalous Hall effect even at zero magnetic field, possibly indicating the presence of chiral edge states. Nonlinearities in $I(V)$ curves at low temperatures suggest a possible role of electronic correlations.

Lucia Steinke received her PhD in physics from the Technical University of Munich, Germany in 2009. After her doctoral research at the Walter Schottky Institute for fundamental research in semiconductor electronics, she worked as a postdoctoral researcher for the Max Planck Institute for Chemical Physics of Solids in Dresden, Germany. She joined Meigan Aronson’s group at Brookhaven National Laboratory in 2014 and in the next year followed Prof. Aronson to her new appointment at Texas A&M University. Lucia’s research interests evolved from novel one-dimensional states along MBE corner-overgrown quantum Hall line junctions to magnetic and multipolar phases in rare-earth intermetallic compounds, as well as magnetism and quantum criticality in transition-metal based compounds. Relating to her PhD work on quantum Hall systems, she recently became interested in topological materials, where she hopes to contribute to the discovery of new topological states and emergent phenomena connected to topological phase transitions.
Pressure-Induced Quantum-Phase Transitions in a Heavy-Fermion Metal

There now are multiple examples of quantum-phase transitions (QPTs) accessed by applying a magnetic field, pressure or both to a heavy-fermion antiferromagnet. In some of these examples, e.g., CeCu$_6$$_{1-x}$Au$_x$ and YbRh$_2$Si$_2$, inconsistencies between experimental observations and theoretical expectations of ‘conventional’ criticality motivated new theoretical concepts to account for measured properties. Unlike the conventional model that is a quantum extension of the theory of thermally-driven phase transitions, these unconventional models invoke criticality of electronic degrees of freedom that may be coincident with magnetic criticality. Measurements, such as Hall effect, deHaas-vanAlphen and thermoelectric power, that are sensitive to the electronic structure have been instructive for identifying unconventional forms of criticality in which a qualitative reconstruction of the Fermi surface is expected. In this talk, I discuss recent thermopower measurements on a derivative of the unconventional quantum-critical material CeRhIn$_5$, the heavy-fermion antiferromagnet CeRh$_{0.88}$Ir$_{0.42}$In$_5$. As pressure is applied to this material, there is a discontinuous jump in thermopower that signals an abrupt Fermi-surface reconstruction at $p_{c1}$, expected of an unconventional QPT, and this is followed by a conventional QPT at $p_{c2}$ across which the Fermi surface evolves smoothly to a heavy Fermi-liquid state. The variation of thermopower with pressure and temperature around these two QPTs is a particularly clear experimental manifestation of theoretical predictions.

Work was performed in collaboration with Y. K. Luo, X. Lu, P. F. S. Rosa, and Q. Si and under the auspices of the U.S. DOE, Division of Materials Sciences and Engineering.

**Thompson** is a Fellow of Los Alamos National Laboratory, the APS and AAAS. His research interest has been the discovery and understanding of new physics in new materials, particularly but not exclusively in rare-earth and actinide heavy-fermion systems under applied pressures.
1. A Non-magnetic Liquid with Nematicity in the Spin-1 SU(3) Heisenberg Model on the Square Lattice

Wen-Jun Hu¹, Shou-Shu Gong², Hsin-Hua Lai¹, Andriy H. Nevidomskyy

¹Department of Physics and Astronomy & Rice Center for Quantum Materials, Rice University, Houston, Texas 77005, USA; ²National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310, USA

We study the spin-1 SU(3) Heisenberg model with the nearest-neighbor bilinear and biquadratic interactions on the square lattice by using the large-scale density matrix renormalization group. By calculating spin and quadrupolar order parameters on the cylinder geometry up to system width L_y=9, we find many competing peaks of structure factor at different momenta including the three-sublattice magnetic order proposed by previous studies. However, through appropriate extrapolation on large system size, all the spin and quadrupolar orders are scaled to zero. Surprisingly, we also find a finite lattice nematicity that characterizes a spontaneous lattice C_4 symmetry breaking. Our results exclude the three-sublattice magnetic order, and reveal a non-magnetic liquid with nematicity in the vicinity of the highly competing SU(3) point. We further discuss this new quantum phase by analyzing the low-energy excitations and by considering different perturbations on the SU(3) model.

2. Effects of Electronic Interactions Near the Topological Semimetal-insulator Quantum Phase Transition in Two Dimensions

Bitan Roy, Matthew S. Foster

The quasiparticle dispersion of gapless excitations residing at the quantum critical point (QCP) separating a two dimensional topological Dirac semimetal and a symmetry preserving band insulator, displays distinct power-law dependence with various components of spatial momenta. First I will review scaling of various thermodynamic and transport quantities at this QCP. Next I will demonstrate that even though such noninteracting QCP is stable against sufficiently weak but generic short-range interaction, the direct transition between the Dirac semimetal and band insulator can either (i) become a fluctuation driven first order transition, or (ii) get eliminated by an intervening broken symmetry phase, with staggered pattern in charge or spin being two prominent candidates, for sufficiently strong interactions. The novel quantum critical phenomena associated with the instability of critical excitations toward the formation of various broken symmetry phases will be presented. Relevance of our study in strained graphene, black phosphorus, pressured organic compounds and oxide heterostructure will be highlighted.

This work was supported by Welch Foundation Grant No. C-1809, NSF CAREER grant no. DMR-1552327.
The metal insulator transition (MIT) in the alloy system $V_{1-x}C_{x}O_3$ has stood as a mystery for many decades [1]. The prevailing model as of 2007, based on dynamical mean field theory (DMFT) calculations, was that of “correlation-enhanced orbital polarization” in which the trigonal crystal field splitting of $t_{2g}$ d-orbitals is driven by many-body effects to the brink of an insulating gap between $e_{πg}$ and $a_{1g}$ orbitals in the metallic phase [2], thus setting the stage for small structural changes to explain the temperature-doping MIT phase diagram. This model of near separation of $t_{2g}$ orbitals, predicts a simple metallic surface of predominantly a single $a_{1g}$ electron pocket at the zone center and completely filled $e_{πg}$ bands. Here the first reported momentum-resolved band structure of metallic phase $V_2O_3$ [3], using angle-resolved photoemission (ARPES), reveals a Fermi surface consistent with near half-filling of the $e_{πg}$ band manifold, incongruous with the above model. This experimentally implied weaker role of orbital polarization in driving the MIT is qualitatively aligned to results of recent DMFT calculations emphasizing full charge self-consistency.

References:

4. High Temperature Heaviness in CeCoIn$_5$
Sooyoung Jang$^1$, J. D. Denlinger$^1$, J. W. Allen$^2$, V. S. Zapf$^3$, M. B. Maple$^4$, Jae Nyeong Kim$^5$, Bo-Gyu Jang$^6$, Ji Hoon Shim$^5$

The temperature-dependent evolution of the Kondo lattice is a long-standing topic of theoretical and experimental investigation and yet it lacks a truly microscopic description of the relation of the
basic f-d hybridization processes to the fundamental $T$ scales of Kondo screening and Fermi-liquid lattice coherence. Here, the $T$-dependence of f-d hybridized band dispersions and Fermi-energy $f$ spectral weight in the Kondo lattice system CeCoIn$_5$ is investigated using $f$-resonant angle-resolved photoemission (ARPES) with sufficient detail to allow direct comparison to first principles dynamical mean field theory (DMFT) calculations containing full realism of crystalline electric field states. The ARPES results, for two orthogonal (001) and (100) cleaved surfaces and three different f-d hybridization scenarios, with additional microscopic insight provided by DMFT, reveal $f$ participation in the Fermi surface at temperatures up to and beyond 200 K, i.e. much higher than the transport lattice coherence temperature, $T^* \approx 45$ K, which is commonly believed to be the onset $T$ for such behavior.

5. Kondo Destruction in an SU(4) Anderson Impurity Model with Bosonic Bath

Ang Cai$^1$, Chia-Chuan Liu$^1$, Emilian Nica$^2$, Rong Yu$^3$, Qimiao Si$^1$

$^1$Rice University; $^2$University of British Columbia; $^3$Renmin University of China

Quantum criticality and Kondo destruction are emerging as a pressing issue in heavy fermion systems with multipole degrees of freedom. Experiment on a metallic system Ce$_3$Pd$_{20}$Si$_6$ under magnetic field has revealed two quantum critical points [1]. One of them has been interpreted as a Kondo destruction associated with the magnetic dipole degrees of freedom [2], and is thought to realize a transition from a small to large Fermi-surface AF$_S$ to AF$_L$ transition in the proposed global phase diagram [3]. Pressure tuned Kondo insulator SmB$_6$ is also found to undergo a quantum phase transition from a Kondo insulating state to a Fermi-liquid state [4]. The four-fold degenerate $\Gamma_8$ crystal field levels in the cubic systems provide a fundamental representation of the SU(4) group. As a minimal model, we analyze the Kondo destruction in an SU(4) symmetric Anderson impurity model, coupled to bosonic baths. We explore the phase diagram using the continuous time Quantum Monte Carlo method. As a function of coupling strength to the bosonic baths, we find that a generic route in the phase diagram will contain two quantum phase transitions: First from both spin and orbital sectors being Kondo screened to one of them being Kondo destroyed, then to both sectors being Kondo destroyed. The implications for experiments will be discussed.

References:
[1] V. Martelli et al., to be published.
6. Quantum Phase Transitions and Anomalous Hall Effect in Frustrated Kondo Lattices

Sarah E. Grefe\(^1\), Wenxin Ding\(^1\), Silke Paschen\(^2,1\), Qimiao Si\(^1\)

\(^1\)Department of Physics and Astronomy & Rice Center for Quantum Materials, Rice University, Houston, TX 77005, USA, qmsi@rice.edu; \(^2\)Institute of Solid State Physics, Vienna University of Technology, Wiedner Hauptstraße 8-10, 1040 Vienna, Austria

Among the pyrochlore iridates, the metallic compound Pr\(_2\)Ir\(_2\)O\(_7\) (Pr-227) has shown characteristics of a possible chiral spin liquid state [1-3] and quantum criticality [4]. An important question surrounding the significant anomalous Hall response observed in Pr-227 is the nature of the f-electron local moments, including their Kondo coupling with the conduction d-electrons. The heavy effective mass and related thermodynamic characteristics indicate the involvement of the Kondo effect in this system’s electronic properties. In this work, we study the effects of Kondo coupling on candidate time-reversal-symmetry-breaking spin liquid states on frustrated lattices. Representing the f-moments as slave fermions Kondo-coupled to conduction electrons, we study the competition between Kondo-singlet formation and chiral spin correlations. We derive an effective chiral interaction between the local moments and the conduction electrons and calculate the anomalous Hall response across the quantum phase transition from the Kondo destroyed phase to the Kondo screened phase. We discuss our results’ implications for Pr-227 and related frustrated Kondo-lattice systems.

References:

7. Skyrmion Defects of Antiferromagnet and its Competing Singlet States in a Kondo-Heisenberg Model

Chia-Chuan Liu\(^1\), Pallab Goswami\(^2\), Qimiao Si\(^1\)

\(^1\)Department of Physics and Astronomy, Rice University, Houston; \(^2\)Condensed Matter Theory Center, University of Maryland, College Park

The competition between antiferromagnetism and a variety of proximate paramagnetic spin-singlet states is a common feature for many heavy fermion compounds, and has been discussed in the proposed global phase diagram [1]. It is important yet a challenging problem to develop a general scheme to access the paramagnetic, spin singlet states from the antiferromagnetically ordered side, and vice versa. In this work, we study the problem on a honeycomb lattice by starting from the Kondo-destroyed antiferromagnetic phase. Here, the local moment is represented by a non-linear sigma model
field, whose topological defects are known to induce the singlet orders based on a perturbative gradient expansion [2]. By solving low energy effective Dirac Hamiltonian in the skyrmion background, we identify the singlet orders through an enhanced correlations in the corresponding channels. In Kondo lattice model, we find two leading singlet channels, one in the spin Peierls sector, and the other in the Kondo singlet sector. The preference of skyrmion defect between spin Peierls and Kondo singlet sector can be changed through tuning the Kondo coupling, causing the crossover between these two sectors in consequence. These results have also been justified by correspondent lattice models. Our results provide new insight into the global phase diagram of the heavy fermion systems.

References:

8. Weyl-Kondo Semimetal in a Heavy Fermion System
Hsin-Hua Lai1, Sarah E. Grefe1, Silke Paschen2,1, Qimiao Si1

1Department of Physics and Astronomy & Rice Center for Quantum Materials, Rice University, Houston, TX 77005, USA, qmsi@rice.edu; 2Institute of Solid State Physics, Vienna University of Technology, Wiedner Hauptstraße 8-10, 1040 Vienna, Austria

The recent observation of Weyl semimetals with negligible interactions makes it pressing to address the role of electron correlations on topological gapless states. With their strong correlations and spin-orbit coupling, heavy fermion systems present a natural setting for such studies. We show that a periodic Anderson model on a noncentrosymmetric lattice realizes a Weyl-Kondo semimetal (WKSM). The quasiparticles near the Weyl nodes involve heavy electrons, which strongly reduces the effective electron velocity near the nodes. Our findings provide the much-needed theoretical foundation for the overall experimental search of f-electron-based Weyl states, and open up a new avenue for systematic studies on correlated topological metals.

References:
9. Transport and Thermodynamic Probes of a Weyl-Kondo Semimetal
Sarah E. Grefe¹, Hsin-Hua Lai², Silke Paschen²,¹, Qimiao Si³

¹Department of Physics and Astronomy & Rice Center for Quantum Materials, Rice University, Houston, TX 77005, USA, qmsi@rice.edu; ²Institute of Solid State Physics, Vienna University of Technology, Wiedner Hauptstraße 8-10, 1040 Vienna, Austria

The spin-orbit coupling and electron correlations of heavy fermion systems make them a rich playground for a variety of quantum phases, including those with topological characteristics. Building upon the recent study of a Weyl-Kondo semimetal phase in the Anderson lattice model in an inversion-symmetry-breaking, three-dimensional model [1], we determine the surface states of the WKSM phase, which feature Fermi arcs, and demonstrate how they manifest the correlation effects. In the strong coupling regime, the quasiparticles near the Weyl nodes have velocities that are strongly reduced by the interaction effects, corresponding to a narrow band, which will make them readily amenable to studies by thermodynamic and thermoelectric means. Here we propose key experimental signatures of the WKSM phase, which are realized in the recently discovered noncentrosymmetric heavy fermion semimetal Ce₃Bi₄Pd₃.

References:

10. Global Phase Diagram of a Kane-Mele-Kondo-Lattice-Heisenberg Model
Xin Li¹,², Rong Yu¹, Tao Xiang¹, Qimiao Si²

¹Institute of Physics, Chinese Academy of Sciences, 100190, China; ²Department of Physics& Astronomy, Rice University, Houston, 77005, USA; ³School of Electrical Engineering and Computer Science, Renmin University of China, Beijing, 100190, China

Motivated by the recent progresses on the topological Kondo insulators, we study the interplay among the spin-orbit coupling, the Kondo coupling, and the RKKY interaction in a Kane-Mele-Kondo-Lattice-Heisenberg model on a two-dimensional honeycomb lattice via a fermionic mean-field theory. We calculated the band structure and chern number of each band on the Kondo–Heisenberg model on honeycomb lattice and investigate the competition between the spin-orbit coupling(SOC) of itinerant electrons and their Kondo coupling with local moments. Further, with the slave-boson applied on the Anderson lattice model, we derived the Kondo hybridization V vary with slave-boson condensation density r under different SOC intensity. We find that the ground-state phase diagram at half-filling contains quite a rich phases, including a topological insulator, a metallic antiferromagnet in absence of Kondo hybridization, and a Kondo insulator. We also identified several competing phases, including a metal with a valence- bond-solid in the spinon sector.

References: