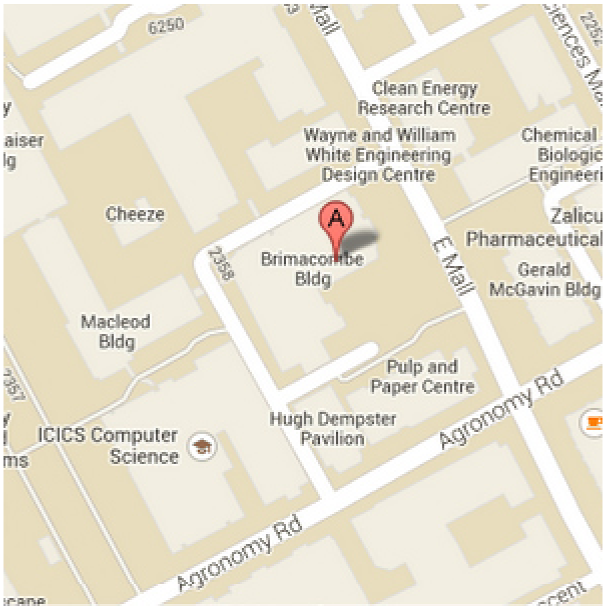
SmB_6 and Related Problems

May 14 – 16 2014

Location:

Brimacombe Building (AMPEL)
Room 311
2355 East Mall Vancouver, BC

Location



UBC Quantum Matter Institute

The Brimacombe Building
111 – 2355 East Mall
Vancouver, BC V6T 1Z4

Tel: (604) 822-3909
Fax: (604) 822-2750
Email: info@qmi.ubc.ca

Quantum
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Institute

QMI is located in the Advanced Materials and Process Engineering Laboratory (AMPEL) in the Brimacombe Building.

Travel Information

By Taxi

A taxi ride from the Vancouver International Airport
to UBC usually takes approximately 30-45 minutes, and costs $30-40 one way

Checker Cab (604) 731-1111
Yellow Cab (604) 681-1111

Public Transit

From Vancouver International Airport, take the Canada Line Skytrain going to Waterfront.

Option 1: Get off at Oakridge-41st Station Northbound. Transfer to either the #43 UBC or #41 UBC buses.

Option 2: Get off at Cambie-Broadway Station Northbound. Transfer to #99 UBC.

Driving Directions

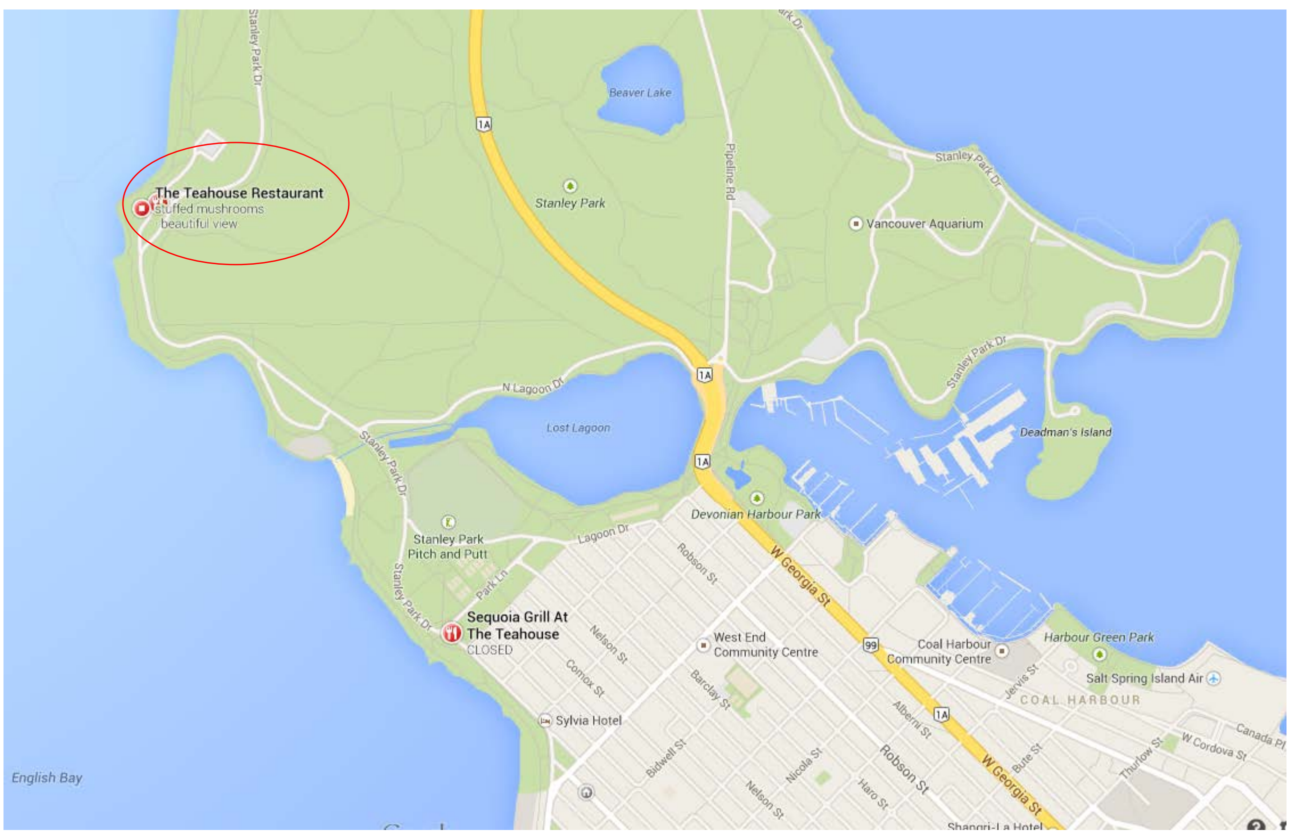
If you are driving from the airport, take Marine Drive to enter UBC, turn right on 16th Ave, in 200 meters turn left on East Mall. Continue driving for 1 kilometer until you see the parking lot.

Parking

There is no free parking on campus. The closest parking lot is the Health Sciences Parkade located across the street from AMPEL.

Restaurant Information

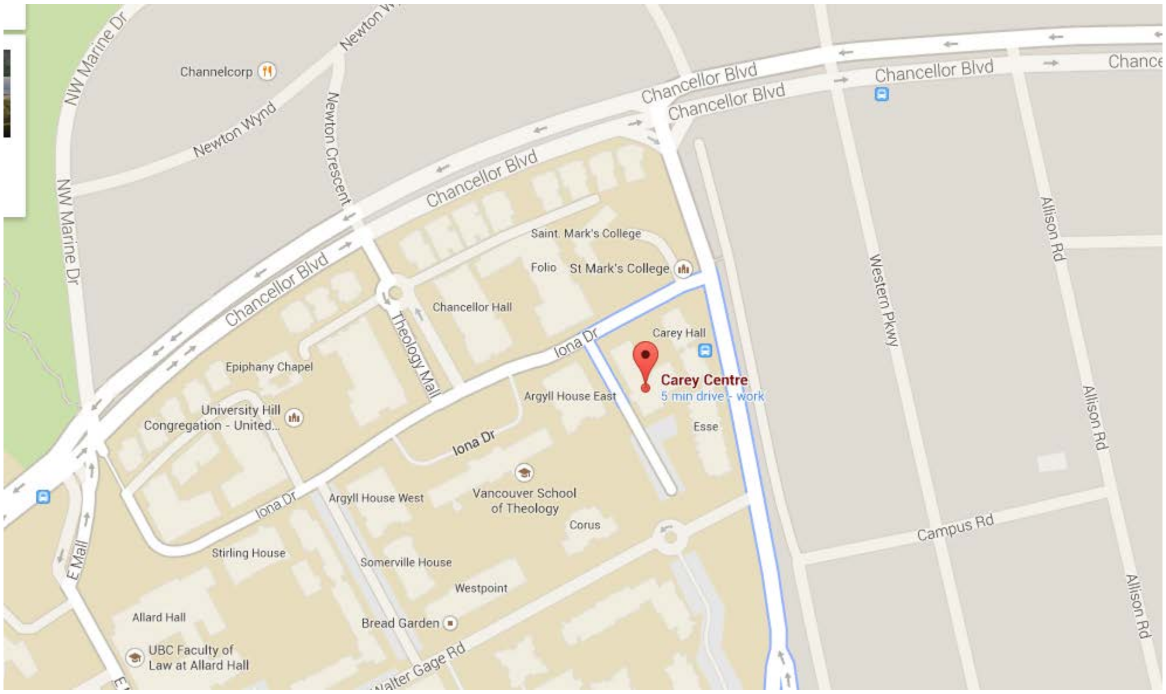
On May 15th, you are cordially invited to a Meeting Dinner at The Tea House in Stanley Park. Round-trip transportation from QMI-UBC is provided. The address is 7501 Stanley Park Dr, Vancouver BC



Accommodation

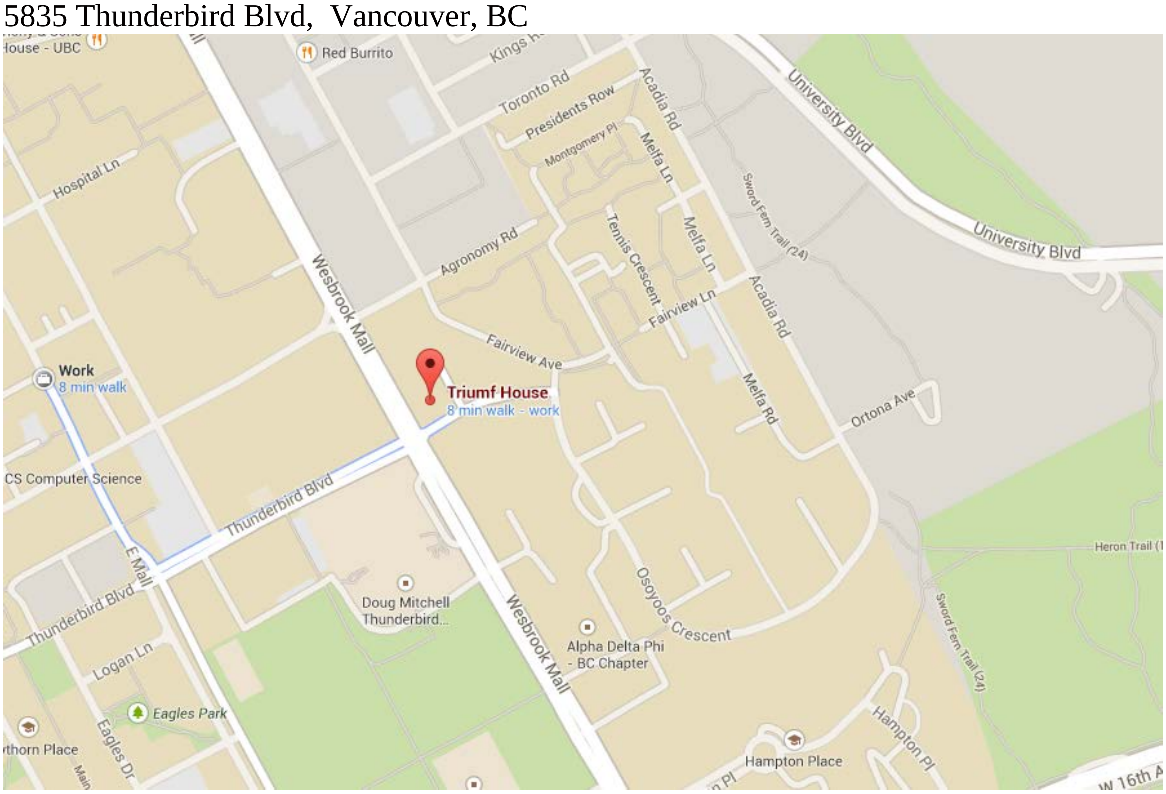
Carey Centre

5920 Iona Dr. Vancouver, BC



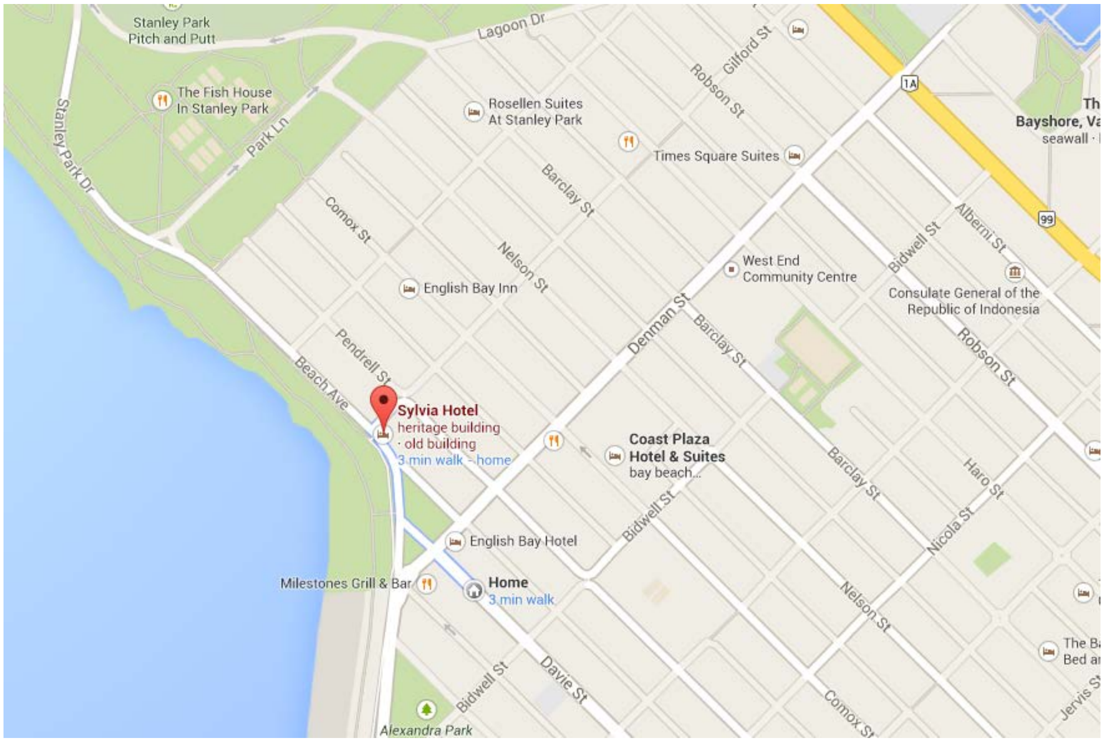
TRIUMF House

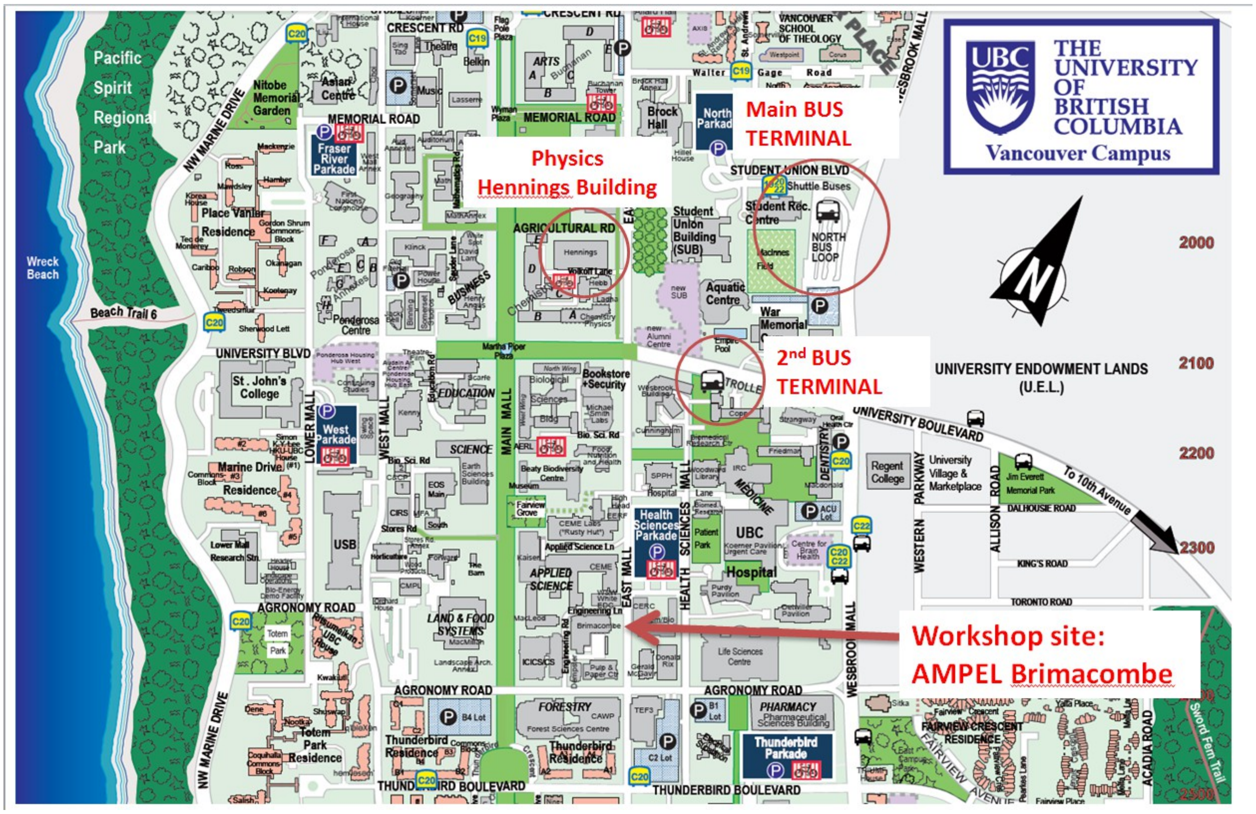
5835 Thunderbird Blvd, Vancouver, BC



Sylvia Hotel

1154 Gilford St. Vancouver, BC

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Vancouver Campus
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Main BUS
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Workshop site:
AMPEL Brimacombe
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Regional
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Wreck
Beach
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NW MARINE DRIVE
MEMORIAL ROAD
CRESCENT RD
AGRICULTURAL RD
STUDENT UNION BLVD
NORTH
BUS
LOOP
UNIVERSITY BLVD
UNIVERSITY BOULEVARD
UNIVERSITY ENDOWMENT LANDS
(U.E.L.)
AGRONOMY ROAD
THUNDERBIRD BOULEVARD
MAIN MALL
EAST MALL
WEST MALL
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HEALTH SCIENCES MALL
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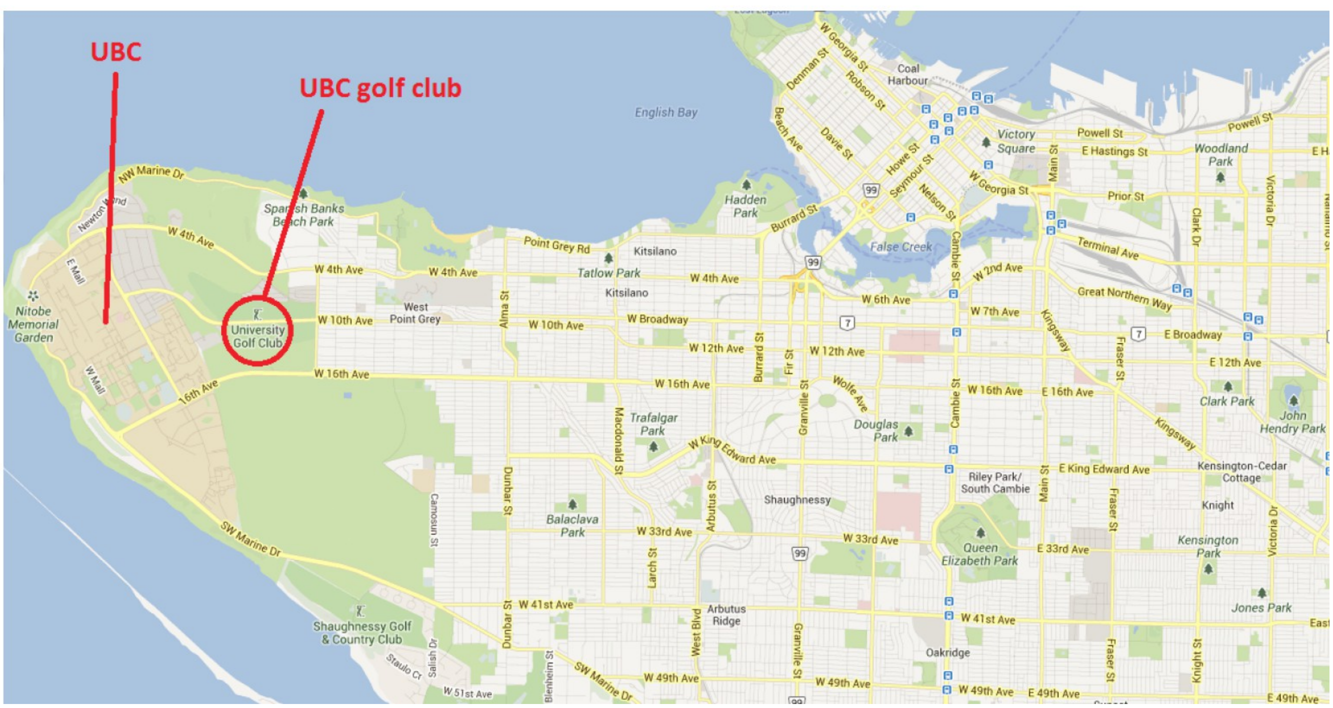
UBC
UBC golf club
University
Golf Club
English Bay
Nitobe
Memorial
Garden
Spanish Banks
Beach Park
Kitsilano
West
Point Grey
Shaughnessy Golf
& Country Club
W 4th Ave
W 10th Ave
W 16th Ave
W Broadway
W King Edward Ave
W 41st Ave
SW Marine Dr
NW Marine Dr

SmB_6 and Related Problems – May 14-16 2014

Room 311 -Brimacombe Building, 2355 East Mall, Vancouver, BC

Time	Wednesday, May 14
9:00 – 9:45 +15 min discussion	**James Allen** (U of Michigan, USA): *SmB6: history and issues*
10:00 - 10:20	Coffee Break
10:20 - 11:00 +15 min discussion	**Vladimir Glushkov** (Prokhorov Phys. Institute, Russia): *Universal features of bulk charge transport and puzzling magnetism of non-metallic hexaborides*
11:15 - 12:30	General Discussion
12:30 - 13:30	Lunch
13:30 – 14:30	**Bernhard Keimer** (Max-Planck, Stuttgart): *Magnetic excitations in CeB6* **Alireza Akbari** (Max-Planck, Stuttgart): *Spin excitons from hybridized heavy quasiparticles*
14:30 - 15:15 +15 min discussion	**Cagliyan Kurdak (**U of Michigan**,** USA**):** *Magnetoresistance Measurements on the Surface States of Samarium Hexaboride using Corbino Structures*
15:30- 16:00	Coffee Break
16:00-16:45	**Johnpierre Paglione** (U of Maryland, USA): *Ferromagnetism and 1D edge state transport in SmB6*
16:45 – 18:00	Discussion
18:00	Enjoy your Evening

Time	Thursday, May 15
8:40- 9:00	James Allen Review of Wednesday's Session *SmB6: history and issues and transport studies*
9:00- 9:45 +15 min discussion	**Lu Li** (U of Michigan, USA*): Quantum Oscillations in Kondo Insulator SmB6*
10:00- 10:30 +15 min discussion	**Ilya Elfimov** (UBC); *Dismembering the band structure of hexaborides and their surfaces with DFT*
10:45- 11:00	Coffee Break
11:00- 11:30 +15 min discussion	**Jennifer Hoffman** (Harvard): *STM imaging of the Kondo Insulating gap of SmB6*
11:45- 12:30	General Discussion
12:30- 13:30	Lunch
13:30- 14:15 + 15 min discussion	**Jonathan Denlinger** (Berkeley Lab, USA): *Temperature-, Photon Energy-, Polarization- and Spatial-dependent Angle-resolved photoemission of SmB6*
14:30- 15:00 +15 min discussion	**Andrea Damascelli** (UBC): *Polarity-Driven Surface Metallicity in SmB6*
15:15- 15:30	Coffee Break
15:30- 16:15 +15 min discussion	**Hao Tjeng** (Max-Planck, Dresden): *Hard x-ray photoelectron spectroscopy on in-situ cleaved and ex-situ polished SmB6 samples; bulk vs. surface electronic structure*
16:30- 17:00 +15 min discussion	**George Sawatzky** (UBC): *4f-4f and 4f,5d multiplets and coulomb and exchange interactions and valence stabilities*
17:15- 18:30	General Discussion
18:45- 22:00	Bus Pickup for transport to Meeting Dinner (2355 East Mall) *Tea House at Stanley Park*

Time	Friday, May 16
9:00 – 9:45 +15 min discussion	**Richard Martin** (U of Illinois): *Bands in rare earth compounds: lessons from SmB6*
10:00- 10:30	Coffee Break
10:30- 11:15 +15 min discussion	**Kai Sun** (U of Michigan, USA): *Topological Kondo insulators and Topological Crystalline Kondo Insulators*
11:30- 12:15 +15 min discussion	**Piers Coleman** (Rutgers, New Jersey, USA) : *Topological Kondo Insulators and SmB6: magnetism meets topology*
12:30- 14:30	Working Lunch with Discussion
14:30- 15:00	Concluding Remarks *End of Workshop*

SmB_6 and Related Problems – May 14-16 2014

Presentation Abstracts

1. **SmB_6: history and issues**
   James Allen

   Wed. May 14, 9:00 – 9:45

Samarium hexaboride SmB_6 is originally famous from more 40 years ago as a mixed valent insulator paradigm flawed by a mysterious resistivity saturation below 4K. All subsequent efforts failed to solve the mystery. Recently SmB_6 has had a huge revival of interest as a new paradigm, now for a new class of strongly correlated topological insulators (TIs), with the predicted topological surface state conduction resolving the long-standing mystery of the residual conductivity. Following the initial theory prediction of this class of “topological Kondo insulators” and experimental evidence for low temperature surface transport, there has been a rush of other studies, both experimental and theoretical, and a concomitant raising of various issues. In fact, very many of these issues were already recognized during the period preceding the current revival of interest, and left in various states of resolution. I will present some of the history of SmB_6 and describe some of these issues.

2. **Universal features of bulk charge transport and puzzling magnetism of non-metallic hexaborides**
   Vladimir Glushkov

   Wed. May 14, 10:20 – 11:00

I present here some selected results of experimental study of charge transport and magnetism in non-metallic hexaborides SmB6, EuB6 and Eu1-xCaxB6 (0≤x≤1).
For SmB6 the origin of intra-gap states, which contribute to conductivity and Seebeck and Hall effects defining the so-called “small gap” below 15K, is briefly discussed. Special attention is paid to the transition into low temperature coherent state below 5K, which is presently believed to be a feature of the non-trivial Z2 topology of the band structure. A signature of spin gap behavior in the magnetic properties of SmB6 allows identifying an extra contribution to magnetic susceptibility, which agrees rather well with the intensity of low-energy excitations detected earlier in neutron scattering (P.Alekseev et al) and Raman spectra (P.Nyhus et al). The possible interference between charge fluctuations and surface states will be discussed as well.
The most interesting puzzle of EuB6 is the extra contribution to spontaneous magnetization. This addition to magnetic moment about 0.4 µB per unit cell appears below percolation transition and increases the saturation moment up to 7.4 µB that exceeds considerably this one for 8S7/2 state of Eu2+ ion. The different approaches are considered to explain this phenomenon in the compound with strong exchange between conduction electrons and localized moments (J~0.1 eV).
Finally, quantum percolation metal-insulator transition in Eu1-xCaxB6 (V.Pereira et al) is shown to induce a huge enhancement of CMR effect (up to ⍰(0)/⍰(7 T)=2.4⍰107 for x=0.36), which follows by the onset of hole conductivity at the border between the metallic and insulating states (xc~0.2). A correlated enhancement of diffusion thermopower, CMR amplitude and Hall coefficient found in the range of 0.15⍰x⍰0.4 points to a smooth change of the band structure under Ca doping. The scaling between resistivity and magnetization found in the paramagnetic phase of Eu1-xCaxB6 is discussed in terms of spin polaronic states, which determine charge transport and CMR enhancement in this strongly correlated electron system.

3. **Magnetic excitations in CeB6**
   Bernhard Keimer

   Wed. May 14, 13:30 – 14:30

We will present inelastic magnetic neutron scattering data on CeB6, a heavy-fermion metal with cubic lattice structure and both antiferromagnetic and antiferro-quadrupolar phases. For a long time, the electronic phase behavior and excitations of CeB6 were described in terms of models based on interacting dipolar and multipolar moments of the localized Ce 4f-electrons. We have recently discovered a prominent excitonic mode akin to the resonant mode in unconventional superconductors that is incompatible with this established perspective. Intense low-energy ferromagnetic magnons further suggest that CeB6 is close to a ferromagnetic instability. These data will be discussed in the context of current theoretical models and related data on other heavy-fermion materials.

References
[1] G. Friemel, Yuan Li, A. V. Dukhnenko, N. Yu. Shitsevalova, N. E. Sluchanko, A. Ivanov, V. B. Filipov, B. Keimer, D. S. Inosov, Nature Communications 3, 830 (2012).
[2] H. Jang, G. Friemel, J. Ollivier, A. V. Dukhnenko, N. Yu. Shitsevalova, V. B. Filipov, B. Keimer, D. S. Inosov, Nature Materials, in press (http://arxiv.org/abs/1308.4491).

4. **Spin excitons from hybridized heavy quasiparticles**
   Alireza Akbari

   Wed. May 14, 13:30 – 14:30

The formation of collective spin excitons below the single particle continuum is observed in numerous unconventional superconductors. $CeCoIn_5$ is the most well established case for heavy fermion compounds. In non-superconducting f-electron compounds the small indirect hybridization gap which is on the scale of the Kondo temperature leads to an enhanced bare spin response around the zone boundary wave vector, Q =(π, π, π). Due to the interaction of hybridized quasiparticles a collective spin exciton resonance mode may appear within or at the gap threshold around Q. It was found in the small hybridization gap semiconductor YbB12 as well as in the heavy fermion metal CeB6. There are similarities to the spin excitons observed within the excitation gap of unconventional superconductors. We use an Anderson lattice type model supplemented by the molecular fields of hidden and magnetic order in the case of CeB6 to calculate the RPA spin response in these compounds. It exhibits the salient feature in frequency and momentum dependence around Q found by inelastic neutron scattering.

5. **Magnetoresistance Measurements on the Surface States of Samarium Hexaboride using Corbino Structures**
   Cagliyan Kurdak

   Wed. May 14, 14:30 – 15:15

Collaborators: S. Wolgast, Y. S. Eo, T. Ozturk, J. Lucien, G. Li, L. Li, K. Sun, and J. W. Allen, *Physics Department, University of Michigan*; D. J. Kim and Z. Fisk, *Department of Physics and Astronomy, University of California, Irvine,* The recent conjecture of a topologically-protected surface state in SmB6 and the verification of robust surface conduction below 4 K have led to a large effort to understand the surface states. Extracting carrier density and charge mobility of these states via Hall measurements is complicated because current can flow on all surfaces of a topological insulator, each of which can have different transport characteristics. We study magnetotransport of SmB6 surfaces up to 45 T using a Corbino geometry that is sensitive to individual surfaces. The Corbino allows us to measure conductivity in both parallel and perpendicular magnetic fields. In the parallel geometry both (110) and (100) samples show a strong negative magnetoresistance at high fields. The conduction on both polar (100) and non-polar (110) surfaces strongly indicates that the conduction must have a non-polarity-driven origin. We have also investigated quantum corrections to conductivity using low-field magnetoresistance measurements. Many of the Corbino samples that we have studied so far have a dip in the magnetoresistance trace that resembles a weak anti-localization feature. The size and temperature dependence of this feature are in general consistent with those expected from a quantum interference correction. However, after careful investigation we found the features shrink in amplitude with slower magnetic field sweep rates. Also, the traces have a hysteretic signal of an unknown origin. The potential coupling between a magnetic oxide layer forming on the surfaces of SmB6 and the topological surface states will be discussed.

Acknowledgements: This project was performed in part at the National High Magnetic Field Laboratory in Tallahassee, FL, and in the Lurie Nanofabrication Facility, a member of NNIN, supported by NSF. This project was funded by NSF grant #DMR-1006500.

6. **Ferromagnetism and 1D edge state transport in SmB6**
   Johnpierre Paglione

   Wed. May 14, 16:00 – 16:45

With hybridization between itinerant conduction electrons and localized f-electrons driving an correlation-induced insulating gap, the Kondo insulator SmB6 is an ideal candidate for realizing the first example of a correlation-derived topological insulator, as predicted by Dzero et al.
We will present low-temperature magnetotransport data that provides evidence for the existence of surface ferromagnetism in SmB6 and proof of the topological nature of metallic surface states. Related work studying magnetic impurity effects, valence state under pressure and related Kondo insulator compounds will be discussed as well.

7. **Quantum Oscillations in Kondo Insulator SmB6**
   Lu Li

   Thu. May 15, 9:00 – 9:45

In Kondo insulator samarium hexaboride SmB6, strong correlation and band hybridization lead to a diverging resistance at low temperature. The resistance divergence ends at about 3 Kelvin, a behavior recently demonstrated to arise from the surface conductance.
However, questions remain whether and where a topological surface state exists. Quantum oscillations have not been observed to map the Fermi surface. We solve the problem by resolving the Landau Level quantization and Fermi surface topology using torque magnetometry. The observed angular dependence of the Fermi surface cross section suggests two-dimensional surface states on the (101) and (100) plane.

Furthermore, similar to the quantum Hall states for graphene, the tracking of the Landau Levels in the infinite magnetic field limit points to -1/2, the Berry phase contribution from the 2D Dirac electronic state.

8. **Dismembering the band structure of hexaborides and their surfaces with DFT**
   Ilya Elfimov

   Thu. May 15, 10:00 – 10:30

I will present our resent density functional calculations of the electronic structure of hexaborides and their surfaces and demonstrate the existence of surface states whose occupation is governed by the degree of surface polarity. We demonstrate that stoichiometric (001) slabs are reconstructed electronically that allows us to deduce the formal valence in these materials. Using model calculations, we demonstrate the rigidity of the basic Boron band structure and show how it is modified due to hybridization between Boron molecular orbitals and cation d states for the energies close to the Fermi energy. The implications of this hybridization for impurity scattering in substituted materials will also be discussed.

9. **STM imaging of the Kondo Insulating gap of SmB6**
   Jennifer Hoffman

   Thu. May 15, 11:00 – 11:30

We use scanning tunneling microscopy to conduct a temperature-dependent, atomically resolved spectroscopic study of the cleaved surface of SmB6. We reveal a robust hybridization gap that universally spans the Fermi level on four different surface morphologies. Employing a cotunneling model, we separate the density of states of the hybridized bands from which the predicted topological surface states must be disentangled. Our technique lays the groundwork for understanding the first strongly correlated topological insulator, and implements a general method to quantitatively understand a wider class of Kondo insulators.

10. **Temperature-, Photon Energy-, Polarization- and Spatial-dependent Angle-resolved photoemssion of SmB6**
    Jonathan Denlinger

    Thu. May 15, 13:30 – 14:15

Temperature-dependent angle-resolved photoemission on cleaved <100> surfaces of SmB6 provides a detailed view of the many-body hybridization gap at the X-point, its destabilization of both valence and conduction band f-states, as well as the intimately connected fate of the robust X-point surface states that reside within the gap. The observed T-dependent evolution agrees very well with bulk transport properties and with the basic predictions of DFT+DMFT calculations, but presently there is no detailed theory for the observed surface state evolution. Spatial variations of the surface state properties on inhomogeneous cleaved surfaces with expected large charge polarity differences between Sm- and B-terminated regions is also explored in comparison to prepared 2x1 reconstructed surfaces.

11. **Polarity-Driven Surface Metallicity in SmB6**
    Andrea Damascelli

Thu. May 15, 14:30 – 15:00

By a combined angle-resolved photoemission spectroscopy and density functional theory study, we discover that the surface metallicity is polarity driven in SmB6. Two surface states, not accounted for by the bulk band structure, are reproduced by slab calculations for coexisting B6 and Sm surface terminations. Our analysis reveals that a metallic surface state stems from an unusual property, generic to the (001) termination of all hexaborides: the presence of boron 2p dangling bonds, on a polar surface. The discovery of polarity-driven surface metallicity sheds new light on the 40-year old conundrum of the low temperature residual conductivity of SmB6, and raises a fundamental question in the field of topological Kondo insulators regarding the interplay between polarity and nontrivial topological properties.

12. **Hard x-ray photoeelectron spectroscopy on in-situ cleaved and ex-situ polished SmB6 samples; bulk vs. surface electronic structure**
    Hao Tjeng

    Thu. May 15, 15:30 – 16:15

Here we report on our on-going electron spectroscopic experiments on SmB6 single crystals to unravel its electronic structure in the bulk as well as in the (near) surface region. We have investigated a crystal which has been cleaved in ultra-high vacuum to obtain a clean surface, as well as a crystal which has been polished and etched under ambient conditions as usually done for samples used in electrical conductivity measurements. This polished and etched crystal was introduced into the spectrometer without further treatment. We have utilized hard x-ray photoelectron spectroscopy (HAXPES) with 6.5 keV photons to achieve probing depths (ca. 80 Angtrom) which are sufficient to obtain spectra that are representative for the bulk material.
By varying the take-off angle away from normal emission we can increase the sensitivity for the surface region. Our temperature dependent (5-300 Kelvin) Sm 3d core level spectra with the characteristic multiplet structures allowed us to reliably determine the valence of the SmB6 in the bulk, with perhaps less ambiguity than the more standard Sm L23 XAS. Preliminary analysis indicates that the Sm valence is about 2.5+ at 5 Kelvin and increases to 2.6+ at 300 Kelvin. The valence band spectrum showed the positions of the 4f5 and 4f4 final states of the bulk with the proper fractional parentages, thereby allowing us to also identify the features in spectra taken with lower photon energies (XPS, UPS, ARPES) which are due to the Sm in the surface.
Astonishing is that the spectra of the polished and etched SmB6 crystal contain very modest oxygen signal, indicating that the SmB6 surface is relatively inert, thus making plausible that reproducible and consistent results can be obtained for the conductivity of the surface region once the bulk part becomes insulating at low temperatures.

13. **4f-4f and 4f,5d multiplets and coulomb and exchange interactions and valence stabilities**
    George Sawatzky

    Thu. May 15, 16:30 – 17:00

I will review some old as well as some new information regarding the Coulomb and exchange interactions and multiplet splittings in general involving 4f -4f and 4f 5d multielectron configurations. Ions with one less or one more than a half filled shell have strongly reduced effective U's for example. I will also discuss the stability of various valence states in general based on the above and on photo and inverse photo emission spectroscopy leading to several elements prone to valence fluctuations or mixed valence states such as Ce 3+,4+, Sm 2+,3+, Eu2+,3+ , Yb 2+,3+. All are elements involved in the interesting discussions at this meeting. I will use several examples from older literature exhibiting features that are special to compounds involving these elements. I will also discuss the importance of the 4f-5d interaction and especially the importance of the ferromagnetic exchange interaction which has for example been directly measured in EuO.

1. Van Der Marel GAS Electron-Electron Interaction and Localization in D and F Transition Metals Phys. Rev. B37, 10674-10684 (1988)
2. J.K.Lang, Y. Baer, P.A.Cox J.Phys. F11, 121 (1981)
3. G. Steeneken, L.H. Tjeng, I. Elfimov, G.A. Sawatzky, G. Ghiringhelli, N.B. Brookes, D.J. Huang, "Exchange splitting and charge carrier spin polarization in EuO", Phys. Rev. Lett. 88, 047201 (2002)

14. Bands in rare earth compounds: lessons from SmB6
Richard Martins

Fri. May 16, 9:00 – 9:45

15. Topological Kondo insulators and Topological Crystalline Kondo Insulators
Kai Sun

Fri. May 15, 10:30 – 11:15

In the study of strongly-correlated insulators, a long-standing puzzle remained open for over 40 years. Some Kondo insulators (or mixed-valent insulators) display strange electrical transport that cannot be understood if one assumes that it is governed by the three-dimensional bulk. In this talk, I show that some 3D Kondo insulators have the right ingredients to be topological insulators, which we called "topological Kondo insulators". For a topological Kondo insulator, the low-temperature transport is dominated by the 2D surface rather than the 3D bulk, because the bulk of this material is an insulator while its surface is a topologically-protected 2D metal. This theoretical picture offers a natural explanation for the long-standing puzzle mentioned above. In addition, we also find that Kondo insulators can support another type of nontrivial topological structure protected by lattice symmetries, which we called "topological crystalline Kondo insulators". In particular, we predict that SmB6 is both a topological Kondo insulator and a topological crystalline Kondo insulator and I will also discuss recent experiments, which reveal the surface states in SmB6.

16. Topological Kondo Insulators and SmB6: magnetism meets topology
Piers Coleman

Fri. May 15, 11:30 – 12:15

The electrons in Heavy fermion materials are subject to spin-orbit coupling nteractions that greatly exceed their Kinetic energy. It has long been known that the spin orbit coupling stablizes new kinds of heavy fermion metals, superconductors and "Kondo insulators" against the competing state of magnetism. I will discuss the latest realization that spin orbit coupling can changing the topology of Kondo insulators, sometimes giving rise to Topological Kondo insulators[2,3] with surface Dirac cones.

We'll specifically discuss SmB6, a KI discovered 45 years ago, predicted to be topological in 2010[2], and tentatively confirmed to be so in a series of experimental studies of the past year[3,4,5]. I'll discuss a simple model for a topological Kondo insulator and briefly introduce the most recent measurements, including ARPES, de Haas van Alphen and weak antilocalization that appear to support the idea that this is a strongly interacting topological insulator. One of the interesting questions is why the surface Dirac Cones seem to involve light fast electrons. I will discuss this in the context of "Kondo Band Bending"- the modification of the Kondo effect by the surface.

[1] Work supported by DOE grant DE-FG02-99ER45790.
[2] M. Dzero et al. Phys. Rev. Lett. 104, 106408 (2010).
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[6] S. Thomas et al. arXiv:1307.4133 (2014).
[7] V. Alexandrov & P. Coleman, arXiv:1403.6819 (2014).