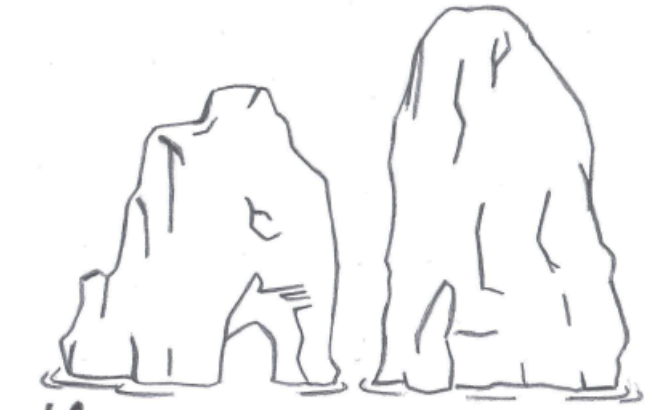

5th Workshop on Complex Oxides

Capri, Italy - May - 20-24-2018

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Programme and abstract book

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Complex oxides have been widely studied in the last decades for the wide range of electronic properties and related intriguing physical phenomena that characterize their phase diagrams. The technical advances in the atomic control of epitaxial synthesis of oxide heterostructures has led to the realization of novel states at their interfaces, such as the creation of quasi two dimensional electron systems, interface superconductivity, quantum Hall effect, multiferroic behavior, novel magnetic orders, often coexisting in the same energy scale. The rich physical properties of complex oxides are also boosting the hopes in an "oxide electronics" in different fields, like novel memories based on resistive switching, spintronics, quantum electronics and energy harvesting.

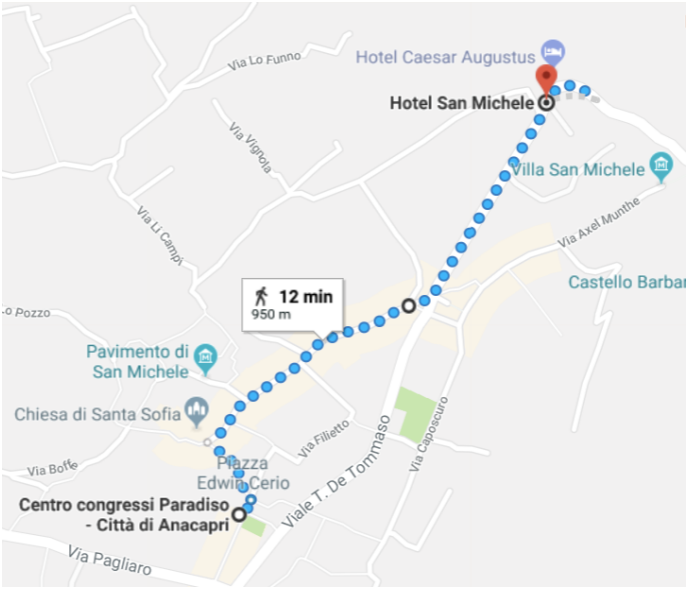
The Workshop on Complex Oxides 2018, is the fifth of the series Initiated in 2010 in Santorini, Greece. The Worskhop moved to Mallorca, Spain in 2012, to Protaras, Cyprus in 2014 and to Porquerolles, France in 2016. The aim of this series of conferences is to gather scientists from all over the world to present recent advances on complex oxides and discuss perspectives for the field.

On behalf of the International and Local Organizing Committees, we welcome you to Capri, wishing you an enjoyable conference in this wonderful island.

WORKSHOP VENUE

The workshop venue is the Centro Congressi Paradiso – Via G. Orlandi, 100, Anacapri.

A special rate for the workshop partecipants has been negotiated with the nearby Hotel San Michele (Via G. Orlandi, 5 – Anacapri) a four star hotel with a marvellous view of the Gulf of Naples and the Sorrento Peninsula.



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Maria Varela
Hyunsoo Yang
Lingfei Wang

5th International Workshop on Complex Oxides, Capri, Italy 20-24 May 2018

		Sunday 20	Monday 21	Tuesday 22	Wednesday 23	Thursday 24		
08:15	08:30		opening				08:15	08:30
			Oxide-2DEGs-1	**Advanced spectroscopy on oxides**	**Magnetism and Spintronics-1**	**Magnetism and Spintronics-3**		
08:30	09:00		Hwang	Fujimori	Barthélémy		08:30	09:00
09:00	09:30		Behnia	King	Yang	Sawa	09:00	09:30
09:30	10:00		Char	Schmitt	Banerjee	Bibes	09:30	10:00
10:00	10:30		Bergeal	Claessen	Santamaria	Panagoupolos	10:00	10:30
10:30	11:00		coffee break	coffee break	coffee break	coffee break	10:30	11:00
			Oxide 2DEGs-2	**Iridates and Topological states**	**Magnetism and Spintronics-2**	**Titanates and novel 2D-oxides**		
11:00	11:30		Fasolino	van der Brink	Shimakawa	Van der Walle	11:00	11:30
11:30	12:00		Salluzzo	Lee	May	Miletto	11:30	12:00
12:00	12:30		Kalaboukhov	Kohno	Wang	Pantelides	12:00	12:30
12:30	13:00		lunch break	Takagi	lunch break	closing	12:30	13:00
				lunch break				
			Advanced structural studies of oxides	free afternoon	**Ferroelectrics and multiferroics**			
15:00	15:30		Dobrosavljevic		Kimura		15:00	15:30
15:30	16:00		Kumah		Iñiguez		15:30	16:00
16:00	16:30		Varela		Gregg		16:00	16:30
16:30	17:00	arrival and registration	Gauquelin		Sando		16:30	17:00
17:00	17:30		coffee break		coffee break		17:00	17:30
			Novel Phenomena in oxides		**Oxide Electronic Devices**			
17:30	18:00		Radovic		Dittmann		17:30	18:00
18:00	18:30		Pentcheva		Huijben		18:00	18:30
18:30	19:00	welcome party	Caviglia		end		18:30	19:00
			end					
	20:00		dinner	dinner	social dinner			20:00

MONDAY, MAY 21

08:15-08:30 OPENING

SESSION 1 – **Oxide 2DEGs -1 (**Chair C. Panagoupulos)

08:30 - 09:00 H. Y. Hwang
3D and 2D Superconductivity in $SrTiO_3$

09:00 - 09:30 K. Behnia
Superconductivity, charge transport and phonon hydrodynamics in strontium titanate

09:30 - 10:00 K. Char
Perovskite oxide heterostructures based on $BaSnO_3$

10:00 - 10:30 N. Bergeal
Superfluid stiffness in oxide interfaces

10:30 - 11:00 coffee break

SESSION 2 – **Oxide 2DEGs – 2 (**Chair M. Radovic)

11:00- 11:30 A. Fasolino
Spin-orbit coupling and Rashba splitting in oxide heterostructures, analogies and differences with semiconductors

11:30 – 12:00 M. Salluzzo
Orbital reconstruction and spin polarization in (100) and (111) LAO/STO and LAO/ETO/STO q2DEG

12:00 – 12:30 A. Kalaboukhov
Superconductivity and magnetism in the nanostructured $LaAlO_3/SrTiO_3$ interface

12:30 – 15:00 lunch break

SESSION 3 – **Advanced structural studies of oxides (**Chair S. Pantelides)

15:00 – 15:30 V. Dobrosavljevic
Critical role of electronic correlations in determining crystal structure of transition metal compounds

15:30 – 16:00 D. Kumah
Stabilizing Magnetism at Polar Oxide Interfaces

16:00 – 16:30 M. Varela
Sub-unit cell mapping of magnetic quantities across complex oxide interfaces

16:30 – 17:00 N. Gauquelin
Structure-property relationships in multi-layered thin films studied by advanced electron microscopy

17:00 – 17:30 coffee break

SESSION 4 – **Novel Phenomena in oxides (**Chair T. Schmitt)

17:30 – 18:00 M. Radovic
Toward the Creation and Control of Properties of Transition Metal Oxides

18:00 – 18:30 R. Pentcheva
Tuning the electronic and thermoelectric response of oxide superlattices by exploiting confinement and interface polarity

18:30 – 19:00 A.D. Caviglia
Berry phase engineering at oxide interfaces

TUESDAY, May 22

SESSION 5 – **Advanced spectroscopy on oxides (**Chair J. Santamaria)

08:30 – 09:00 A. Fujimori
Magnetic anisotropy of ferromagnetic oxide thin films studied by angle-dependent XMCD

09:00 – 09:30 P.D.C. King
Maximal Rashba-like spin splittings and intrinsic Stoner instabilities at polar surfaces of delafossite oxides

09:30 – 10:00 T. Schmitt
Resonant Inelastic X-Ray Scattering on Confined Vanadates and Strained Iridate Films

10:00 – 10:30 R. Claessen
Dimensionality-driven metal-insulator-transition in spin-orbit coupled $SrIrO_3$

10:30 – 11:00 coffee break

SESSION 6 – **Iridates and topological states (**Chair R. Claessen)

11:00 – 11:30 J. van der Brink
Iridates and $RuCl_3$ - from Heisenberg antiferromagnets to potential Kitaev spin-liquids

11:30 – 12:00 H.N. Lee
Quantum phenomena in correlated spin-orbit coupled oxide heterostructures

12:00 – 12:30 H. Kohno
Theory of Topological Hall Effect: From Strong to Weak Coupling

12:30 – 13:00 H. Takagi
Exotic spin-orbital entangled states in 4d and 5d complex oxides

13:00 – 15:00 lunch break

free afternoon

WEDNESDAY 23 MAY

SESSION 7 – **Magnetism and Spintronics – 1 (**Chair M. Bibes)

08:30 – 09:00 A. Barthélémy
Spinorbitronics in engineered $SrTiO_3$-based 2-dimensional electron systems

09:00 – 09:30 H. Yang
Oxide heterostructure based magneto-transports

09:30 – 10:00 T. Banerjee
Emergent functionalities at oxide heterointerfaces induced by spin orbit interactions

10:00 – 10:30 J. Santamaria
Oxygen vacancy controlled functionalities in multiferroic tunnel junctions

10:30 – 11:00 coffee break

SESSION 8 – **Magnetism and spintronics – 2 (**Chair F. Miletto Granozio)

11:00- -11:30 Y. Shimakawa
Charge and spin transitions in perovskite-structure oxides containing unusually high-valence Fe

11:30 – 12:00 S.J. May
Functional Properties of $CaFeO_3$ and $SrFeO_3$ Heterostructures

12:00 – 12:30 L. Wang
Ferroelectrically tunable magnetic skyrmions in ultrathin oxide heterostructures

12:30 – 15:00 lunck break

SESSION 9 – **Ferroelectrics and multiferroics (**Chair M. Huijben)

15:00 – 15:30 T. Kimura
Magnetoelectric multi-spin variables in complex transition-metal oxides

15:30 – 16:00 J. Íñiguez
Polar metals, ferroelectric metals

16:00 – 16:30 J.M. Gregg
Ferroic Domain Walls for Transient Nanoelectronics and Phononics

16:30 – 17:00 D. Sando
Tuning functional properties of $BiFeO_3$ films using strain and growth chemistry

17:00 – 17:30 coffee break

SESSION 10 – **Oxide electronic devices (**Chair A. Sawa)

17:30 – 18:00 R. Dittmann
Uncovering switching and failure mechanism in memristive devices by operando spectromicroscopy

18:00 – 18:30 M. Huijben
Enhanced lithium transport in highly ordered complex oxide cathode films towards solid-state batteries

THURSDAY 24 May

SESSION 11 – **Magnetism and spintronics-3** (Chair A. Barthélémy)

09:00 – 09:30 A. Sawa
Highly Stable Artificial STDP Synapse Based on Oxide FET

09:30 – 10:00 M. Bibes
Imaging, controlling and harnessing non-collinear magnetism in perovskite oxides

10:00 – 10:30 C. Panagoupolos
Electronic transport and microscopic imaging at oxide interfaces

10:30 – 11:00 coffee break

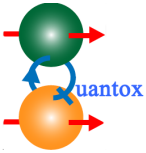
SESSION 12 – **Titanates and novel 2D oxides** (Chair M. Salluzzo)

11:00 – 11:30 C.G. Van der Walle
Electronic and optical properties of rare earth titanates

11:30 – 12:00 F. Miletto-Granozio
Charge Transfers Across Oxide Interfaces Hosting a 2-Dimensional Electron Gas

12:00 – 12:30 S. Pantelides
Square-lattice TMO monolayers and Van der Waals heterostructures

12:30 – 13:00 closing



QUANTOX: QUANtum Technologies with 2D-OXides

One of the most fascinating challenges in solid-state physics in the recent years is the search for Majorana fermions, which take their name from the Italian physicist Ettore Majorana, who theorized their existence at the beginning of the 20th century. These particle-like objects can emerge from interactions in materials characterized by exotic topological properties. Thouless, Haldane and Kosterlitz won the 2016 Nobel Prize in Physics for their theoretical study of topological phases in two-dimensional materials. A qubit working through the control of Majorana particles would be insensitive to decoherence, solving one of the main problems of quantum computation.

QUANTOX proposes a novel material platform for the realization of topological quantum computers: two-dimensional electron gas (2DEG) formed at the junction between insulating oxides, namely $LaAlO_3$ and $SrTiO_3$. This platform has all the characteristics for the practical realization of theory-based proposals for topological quantum computation, and fundamental and technological advantages, like the possibility to scale the technology to complex systems and to include a large number of qubits in a seamless way.

The project is lead by the Italian CNR-SPIN institute and joins together theoretical and experimental groups among the most active in the physics of oxide 2DEGs in the extended European Research Area, including experts in Majorana Physics and topological quantum computation.

It is aimed at establishing oxide 2DEGs as a viable platform for the realization of topological quantum computers, thus launching a new technological approach to the realization of "fault tolerant" quantum computation technology.

For more information, visit the QUANTOX website: www.quantox.spin.cnr.it

Quantox Consortium

Country	Institution/ Department	Name of the Principal Investigator (PI)
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SWEDEN	CHALMERS	A. Kalaboukhov
FRANCE	CNRS-THALES	M. Bibes
SPAIN	UCM	J.Santamaria
FRANCE	ESPCI	N. Bergeal
ISRAEL	BIU	B. Kaliski

Superconducting technologies are prime candidates to ripen quantum effects into devices and applications. In the latest years, a new field has emerged where quantum behavior is controlled by using hybrids of superconductors with magnets, insulators, semiconductors or normal metals. The field will impact crucial areas for societal development, including energy, transport, medicine or computation.
The scientific and technical communities working in superconductivity, whose activities put Europe at the frontier of research, are traditionally small groups working independently. The NANOCOHYBRI Action aims to address the pressing need for a common place to share knowledge and infrastructure and develop new cooperative projects. To this end, we have set-up a program including networking activities with an open, proactive and inclusive approach to other researchers and industry. This will improve availability of infrastructure and knowledge, avoiding duplication of resources and skills and with a focus on contributing to gender balance and the participation of young researchers.

The NANOCOHYBRI Action started in November 2017 and will last until October 2021. Currently, 24 countries have joined the Network. A key objective is to provide training and career development opportunities to Early Career Investigators (ECIs – are those who have completed their PhD degree within the last 8 years). We offer networking opportunities, give publicity to your publications, allow to present ongoing research and to contribute to a large scale project of topical interest. Our instruments include:

- Training schools
- Short-term Scientific Missions (STSMs)
- Early career investigator Conference grants

For more information, please visit the NANOCOHYBRI website:

http://nanocohybri.eu/

Solid State Actuators for Micro/Nanorobotics

Micromechanical actuators have enormous applicative potential in numerous technologies such as microfluidics, drug delivery, artificial muscles, opto/micromechanical switches. Actuation at microscopic scale is mainly performed electrically through capacitive couplings and piezoelectrics or thermally (electrothermally or light irradiation), exploiting the change of shape of specific materials (i.e. Shape Memory Alloys, SMA) or thermal expansion (bimorphs). Best performances are characterized by high relative elongation, large force output and high actuation speed. Vanadium dioxide (VO_2) has been recently considered as an optimum active material in micro/nanoactuators, due to its fast (ps) and sharp solid state phase transition (SSPT) nearby 68°C from monoclinic (M1-M2) phases to the rutile type tetragonal (R) phase that in single crystal can produce strain up to 1% and large applied forces [K. Liu et al. Adv. Mater. 2014, 26, 1764]. This SSPT is accompanied by a Metal-Insulator Transition with a large change (up to 4 orders of magnitude) of electrical resistivity. In this project, we setup strategies for the development of thin film actuators and resonant devices based on the SSPT of VO_2. We plan to establish the scalability limits and the advantages of this technology with respect to the existing state-of-the-art. We aim at realizing micro/nanomechanical devices exploiting the change of lattice parameters of VO_2 thin film nanostructures upon heating. Although energy efficiency of thermal-based actuation schemes is generally low, thermal actuation at nanoscale can be particularly interesting due to the easiness of fabrication associated with large applied force.

This project is coordinated by the CNR-SPIN institute and by ISIR-Osaka University and is supported by the Executive programme of cooperation between Italy and Japan by the Directorate General for Cultural and Economic Promotion and Innovation of the Ministry of Foreign Affairs and International Cooperation, of the Italian Republic. The activity on VO_2 is also sponsored by the CNR-JSPS joint research projects 2018-2019, bilateral agreements of Scientific and Technological Cooperation.

For more information, visit the VO_2 actuator website:
www.vo2actuators.spin.cnr.it

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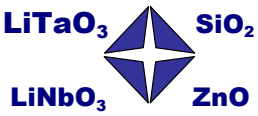

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ABSTRACTS

3D and 2D Superconductivity in $SrTiO_3$

H. Y. Hwang[1,2]
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[2]SLAC National Accelerator Laboratory, Menlo Park, CA, USA
E-mail: hyhwang@stanford.edu

The nature of superconductivity in the dilute semiconductor $SrTiO_3$ has remained an open question for over half a century. Furthermore, recent developments in thin film heterostructures provide new opportunities to examine $SrTiO_3$ superconductivity in reduced dimensions. Here we present work on two aspects of this problem.

In 3D, we take advantage of a newly developed method for engineering band alignments at oxide interfaces and access the electronic structure of Nb-doped $SrTiO_3$ using high-resolution tunneling spectroscopy [1]. While we observe strong coupling to the highest-energy longitudinal optic (LO) phonon consistent with $\lambda \sim 1$, the superconducting gap is found to be in the weak-coupling limit of BCS theory, i.e. $\lambda_{BCS} \sim 0.1$. This discrepancy arises in the context of an unusual anti-adiabatic condition for superconductivity in $SrTiO_3$, here with the Fermi energy < Debye energy.

In 2D, we examine the superconducting $LaAlO_3/SrTiO_3$ interface in devices with dual electrostatic gates [2], which give independent control of the carrier density and effective disorder strength over a wide range. We find a 2D superconducting dome as a function of the dual gate voltages at base temperature, and in all measureable directions, the superconducting phase is bounded by transitions into an unconventional metallic phase characterized by phase fluctuations between superconducting puddles.

References

[1] A. G. Swartz, H. Inoue, T. A. Merz, Y. Hikita, S. Raghu, T. P. Devereaux, S. Johnston, and H. Y. Hwang, PNAS **115**, 1475 (2018)
[2] Z. Y. Chen, A. G. Swartz, H. Yoon, H. Inoue, T. A. Merz, D. Lu, Y. W. Xie, H. T. Yuan, Y. Hikita, S. Raghu, and H. Y. Hwang, in review

Superconductivity, charge transport and phonon hydrodynamics in strontium titanate

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Long-range ferroelectric order is aborted in strontium titanate because of quantum fluctuations. As a consequence, the low-temperature static electric permittivity becomes extremely large and the effective Bohr radius of the order of a micron. This is why removing a tiny fraction of oxygen atoms turns the system to a dilute metal, which has both a sharp Fermi surface and a superconducting instability [1]. Substituting strontium with calcium stabilizes a long-range ferroelectric order in $Sr_{1-x}Ca_xTiO_3$ coexisting with metallicity and its superconducting instability in a narrow window of doping. As the carrier concentration is increased, the ferroelectric order is eventually destroyed by a quantum phase transition and the superconducting critical temperature is enhanced [2]. Recent analysis points to the failure of Boltzmann-Drude picture of conductivity in explaining charge transport of this dilute metal [3]. Thermal transport in the insulator detects the Poiseuille flow of phonons in a narrow temperature window as a consequence of strong coupling between the ferroelectric soft mode and acoustic phonons [4].

References

[1] X. Lin *et al.,* Phys. Rev. Lett. **112**, 207002 (2014)
[2] C. W. Rischau *et al.,* Nature Phys. **13**, 643 (2017)
[3] X. Lin *et al.,* NPJ Quantum Materials **2,** 41 (2017)
[4] V. Martelli *et al*., Phys. Rev. Lett. **120**, 125901 (2018)

Perovskite oxide heterostructures based on $BaSnO_3$

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A wide-bandgap perovskite oxide semiconductor $BaSnO_3$ was recently found to possess high mobility and excellent stability. Its single crystal mobility value of about 300 $cm^2/V{\cdot}sec$ in the doping range of 10^{19}~$10^{20}/cm^3$, when n-type La dopants in place of Ba are used, is the highest among all the semiconductors. Furthermore, the oxygen diffusion constant in $BaSnO_3$ was measured to be several orders of magnitude lower than 3d transition metal perovskite oxides, demonstrating superb stability of the material.

Taking advantage of such properties, excellent field effect transistors were recently demonstrated using amorphous gate oxides (AlO_x and HfO_x) as well as high-k epitaxial gate oxides such as $LaInO_3$ and $BaHfO_3$, which led to development of an all-perovskite transparent high mobility field effect transistor. In addition, p-type doping by K in place of Ba is feasible and the pn-junctions made with K-doped $BaSnO_3$ and La-doped $BaSnO_3$ were demonstrated to exhibit near-ideal IV characteristics. Moreover, 2DEG behavior is found at the polar interface of $BaSnO_3$ and $LaInO_3$. We will go over the parameters that control the 2DEG behavior and discuss the mechanism behind such behavior.

In spite of these tremendous progresses, the device performances are currently limited by defects such as threading dislocations. Once all the major defects are removed, the perovskite oxide semiconductor $BaSnO_3$ system, especially when it is combined with other perovskite oxides, is expected to offer much more opportunities for science and technology.

Superfluid stiffness in oxide interfaces

G. Singh[1,2] , A. Jouan[1,2], L. Benfatto[3,4], F. Couedo[1,2], P. Kumar[5] , A. Dogra[5], R. Budhani[6], S. Caprara[3,4], M. Grilli[3,4], E. Lesne[7], A.Barthelemy[7], M. Bibes[6], C. Feuillet-Palma[1,2], J. Lesueur[1,2], and N. Bergeal[1,2]

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The discovery of a gate-tunable 2D superconducting electron gas [1] in oxide hetero-interfaces in coexistence with both ferromagnetism [2] and a strong Rashba spin-orbit coupling [3], has raised a considerable interest. However, the evolution of fundamental parameters with electrostatic doping, such as the pairing strength between electrons (i.e. the gap energy Δ) is non trivial [4]. We will present recent resonant microwave transport measurements on $LaAlO_3/SrTiO_3$ interfaces that allows extracting the superfluid stiffness Js, i.e. the energy scale which determines the cost of a phase twist in the superconducting condensate. We find that the competition between Js and Δ controls the superconducting phase diagram obtained by plotting the superconducting Tc as a function of gate voltage. Whereas a good agreement with the Bardeen-Cooper-Schrieffer (BCS) theory is observed at high carrier doping, our data suggest that the suppression of Tc at low doping is controlled by the loss of macroscopic phase coherence instead of electron pairing as in standard BCS theory. The analysis of the superfluid density also reveals that only a very small fraction of the electrons condenses into the superconducting state, which we relate to the filling of specific orbitals in the interfacial quantum well [5].

References

[1] A. D. Caviglia *et al.*, Nature **456**, 624 (2008)
[2] J. Bert *et al.*, Nature Phys. **7**, 767771 (2011)
[3] A. D. Caviglia *et al.*, Phys. Rev. Lett. **104**, 126803 (2010)
[4] C. Richter *et al.*, Nature **502**, 528531 (2013)
[5] G. Singh *et al.*, Nat. Commun. **9**, 407 (2018)

Spin-orbit coupling and Rashba splitting in oxide heterostructures, analogies and differences with semiconductors

L. W. van Heeringen[1], G. de Wijs[1], A. McCollam[1], J. C. Maan[1], and A. Fasolino[1]

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The band structure of oxide heterostructures suggests that approaches that have been successful for semiconductor heterostructures can become relevant for this new class of materials. In particular, for STO, strong spin-orbit coupling deeply affects the free electron character of the bulk electronic bands, such that they can be theoretically described in ways analogous to the hole bands in III-V semiconductors [1-2]. Recently, many experimental results have addressed the Rashba spin splitting due to asymmetry at the interfaces in oxide heterostructures in the presence of spin-orbit coupling. Rashba spin splitting in two-dimensional (2D) semiconductor systems is generally calculated in a $\mathbf{k} \cdot \mathbf{p}$ Luttinger-Kohn approach where the spin splitting due to asymmetry emerges naturally from the bulk structure. In oxides heterostructures, instead, the effects of asymmetry leading to Rashba splitting have typically been treated phenomenologically. We compare the effect on a given conduction band structure of these two descriptions of the Rashba spin splitting that have been developed independently in the two fields of semiconductors and correlated electrons and find that the two models produce fundamentally different behavior in regions of the Brillouin zone that are particularly relevant for magnetotransport.

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Orbital reconstruction and spin polarization in (100) and (111) LAO/STO and LAO/ETO/STO q2DEG

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In the last decade, the tremendous advances in the atomic-scale deposition of transition metal oxides have led to the discovery of novel functional electronic and magnetic properties at the oxide interfaces. One of the most important example is the discovery of a quasi-two-dimensional electron gas (q2DEG) at the interface between (001) $SrTiO_3$ (STO) single crystals and $LaAlO_3$ (LAO) [1].

Some of the distinctive properties of the (001) LAO/STO system arise from the occurrence of an orbital reconstruction, first demonstrated by x-ray linear dichroism (XLD) [2] and later on by Angle Resolved Photoemission Spectroscopy (ARPES) [3]. The orbital reconstruction causes a reverse ordering and splitting of the bulk conduction bands derived by non-degenerate t_{2g} (3dxy, 3dxz, 3dyz) orbitals of Ti3d-states with D4h (tetragonal) crystal field. A similar orbital reconstruction is observed in delta doped (001) LAO/ETO/STO heterostructures, which have the interesting property to form a q2DEG characterized by a superconducting ground state and a spin-polarization [4].

In this talk I will present an overview of the electronic and magnetic properties of both (001) and (111) LAO/STO and LAO/ETO/STO q2DEG as investigated by x-ray spectroscopy, including x-ray absorption spectroscopy, x-ray linear and magnetic dichroisms and angle resolved photoemission. The results are compared to transport and magneto-transport properties of the system.

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Superconductivity and magnetism in the nanostructured $LaAlO_3/SrTiO_3$ interface

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The interface between wide band-gap insulators, $LaAlO_3$ and $SrTiO_3$ (LAO/STO) has received much attention since it possesses very exciting electrical properties such as a quasi-two-dimensional electron gas (q2DEG), two-dimensional superconductivity, ferromagnetic behavior and giant spin-orbit coupling [1]. Coexistence of ferromagnetic ordering and superconductivity is one of the most intriguing aspects for the LAO/STO interface. There are also indications that the superconducting state is inhomogeneous on nanoscale [2]. In order to gain better understanding of the ground state of the LAO/STO interface, we have systematically investigated superconductivity in the nanostructureds with dimensions of 100 – 300 nm [3]. The nanostructures were fabricated using our patterning method based on low-energy Ar+ ion beam irradiation [4]. We realized nano-rings and nano-wires with a lateral width of 100 – 300 nm. Analysis of current-voltage characteristics suggests that our nanostructures behave like clean superconducting filaments without formation of weak links. Moreover, we observed a SQUID-like periodic modulation of the critical current in nano-rings corresponding to the Little-Parks fluxoid quantization. A most remarkable observation is an enhancement of the critical current by a small perpendicular magnetic field. This effect may be explained by the suppression of spin flip scattering on magnetic domains by external magnetic field [5] or by induced unconventional pairing [6]. The nature of magnetic ordering in the LAO/STO interface is still elusive that complicates the interpretation of the superconducting transport properties. We will review some possible experimental configurations that would allow unequivocal determination of the superconducting ground state at the LAO/STO interface.

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Critical role of electronic correlations in determining crystal structure of transition metal compounds

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The choice that a solid system ”makes” when adopting a crystal structure (stable or metastable) is ultimately governed by the interactions between electrons forming chemical bonds. By analyzing 6 prototypical binary transition-metal compounds we demonstrate [1] here that the orbitally-selective strong d-electron correlations influence dramatically the behavior of the energy as a function of the spatial arrangements of the atoms. Remarkably, we find that the key physical mechanism underlying this complex behavior can be traced back to simple electrostatics, i.e., to the fact that the strong d-electron correlations influence substantially the charge transfer mechanism, which, in turn, controls the electrostatic interactions. This result advances our understanding of the influences of strong correlations on the crystal structure, opens a new avenue for extending structure prediction methodologies to strongly correlated materials, and paves the way for predicting and studying metastability and polymorphism in these systems.

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Stabilizing Magnetism at Polar Oxide Interfaces

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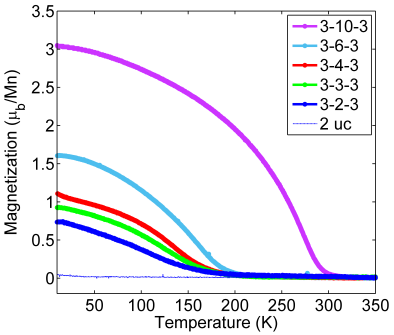
Atomic-scale interactions at the interfaces between polar and non-polar transition metal oxides have led to the realization exciting phenomena including two-dimensional electron gases and interfacial magnetism. However, these interactions may lead to the suppression of electronic and magnetic ordering at interfaces with strong structure-property relationships. By imaging the atomic structure of the interface between polar $LaSrMnO_3$ (LSMO) and non-polar $SrTiO_3$, we identify interfacial structural distortions which are correlated with thickness-dependent metal-insulator and ferromagnetic-paramagnetic transitions in the rare-earth manganites. We show that these structural distortions can be tuned by inserting polarity-matched spacer layers at the LSMO interfaces leading to a stabilization of ferromagnetism in LSMO layers as thin as two unit cells. The stabilized magnetism is found to be independent of strain. We employ a combination of synchrotron X-ray diffraction, temperature-dependent magnetization measurements and X-ray magnetic circular dichroism to elucidate the interplay between structural and spin degrees of freedom in the rare-earth manganites.[1,2] These results demonstrate the intimate role of picometer-scale structural distortions on the physical properties of transition metal oxides and have important implications for confining magnetism to two-dimensions in ultra-thin oxide films.



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Sub-unit cell mapping of magnetic quantities across complex oxide interfaces

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Magnetic oxides with perovskite structure exhibiting colossal magnetoresistance are very relevant systems from the point of view of both physical properties and technological relevance. This talk will discuss local measurements of electronic and magnetic properties of ferromagnetic manganite $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) epitaxial ultrathin films grown by high-pressure O_2 sputtering on single crystal $SrTiO_3$ (STO) substrates. We will combine the use of advanced electron microscopy techniques such as electron energy-loss spectroscopy (EELS) in the aberration-corrected scanning transmission electron microscope (STEM) with density-functional calculations to study local structural distortions and electronic phenomena associated with interfacial magnetism. Atomic resolution images exhibit an increase of the out-of-plane lattice parameter at the LSMO/STO interface plane, pointing to a local reconstruction of the charge density and, hence, physical properties. We use energy-loss magnetic chiral dichroism (EMCD) [1,2], a technique directly sensitive to the local magnetic moment, to track magnetic quantities across the interface with sub-unit cell resolution. The dichroic signal at both the Mn $L_{2,3}$ and the Ti $L_{2,3}$ edges is enhanced near the interface, pointing to a local increase of the Mn and Ti magnetic moments. These results agree with density-functional theory simulations including interfacial oxygen vacancies, which enhance charge transfer and antiferromagnetic coupling between the Ti and the Mn.

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Structure-property relationships in multi-layered thin films studied by advanced electron microscopy

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The study of novel physical properties appearing when two materials are interfaced has become one of the major fields of research in solid-state physics over the last decade. As the materials involved in those new physical phenomena are often complex oxides, many factors (such as strain, oxygen stoichiometry, cation intermixing, electronic reconstructions) have to be considered when discussing their origin. If the two interfaced materials have different octahedral tilt systems, one has to adapt to the other. Electron microscopy imaging (HAADF, ABF) and EELS spectroscopy are key tools for their study.

I will be reporting recent results enlightening the effect of oxygen octahedral coupling on the change of the magnetic easy-axis in some ferromagnetic manganite films. [1] The relationship between this change of magnetism and the change in hybridization between the metal and the oxygen orbitals will be presented [2,3]. A second part of the presentation will be focused on rare-earth nickelate perovskites $RNiO_3$ (R being the rare earth) which possess a metal-insulator transition (MIT) that is tuneable in the bulk by the size of the rare-earth atom, sitting on the A site, which influences the rotation of the NiO6 octahedra.[4] In thin-film heterostructures, the rotation patterns can be altered by epitaxial strain. In this contribution recent results that show that the oxygen octahedral rotations of a given compound can be precisely adjusted within a broad range by combining $SmNiO_3$ with a different perovskite used as a tilt-control layer (TCL) will be presented.

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Toward the Creation and Control of Properties of Transition Metal Oxides

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Transition Metal Oxides (TMOs) exhibit unique and multifunctional physical phenomena (such as high-temperature superconductivity, colossal magnetoresistance, metal-insulator transitions, etc.) directly related to the spin and orbital degrees of freedom of the transition metal d-states and their interplay with the lattice. Importantly, the iso-structure of TMOs permits realization of hetero-structures generating at their surfaces and interfaces new physical matters that radically differ from those of the constituent bulk materials.
Through two examples, novel and fascinating properties emerged in TMO based hetero-structures and ways to control them will be presented:

1. Altering orbital ordering and band filling of the 2DEG at titanates surfaces. Employing ARPES we found ways to manipulate the 2DEG and, consequently, to tune electronic properties of titanates surfaces ($SrTiO_3$ in bulk and film forms [1], TiO_2-anatase [2] and $CaTiO_3$ [3] films).

2. Tuning electronic phases in ultra-thin $NdNiO_3$ (NNO) and $SrIrO_3$ (SIO) films via the proximity to the magnetic layer.
The electronic structure of NNO and SIO films grown solely and in proximity to magnetically ordered manganite layers has been studied. We found that the insulator ground phase in ultra-thin NNO films is destabilized probably due to quenching of antiferromagnetic (AF) order via proximity to the ferromagnetic manganite layer [4,5].

Over-all studies establish different approaches to manipulate the properties of the two-dimensional electron gas and electronic phases signifying perspectives of TMO for novel applications.

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Tuning the electronic and thermoelectric response of oxide superlattices by exploiting confinement and interface polarity

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Oxides are a promising materials class for thermoelectric applications due to their chemical and thermal stability and environmental friendliness. Nanostructuring and reduced dimensionality promise further optimization of the thermoelectric response [1]. By combining DFT+*U* calculations and Boltzmann transport theory we explore the implications of interface polarity and confinement on the thermoelectric properties of nickelate superlattices. Taking as an example $LaNiO_3/SrTiO_3$(001) superlattices, we demonstrate that compatible *n*- and p-type materials can be realized by selective choice of the layer stacking at the polar interfaces [2]. On the other hand, a strongly enhanced thermoelectric response is obtained in $LaNiO_3/LaAlO_3$(001) superlattices due to confinement [3]. Last but not least we discuss the effect of localized electrostatic doping in La_2CuO_4/ $LaNiO_3$(001) superlattices is discussed [4].

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Berry phase engineering at oxide interfaces

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Geometric phases in condensed matter play a central role in many intriguing phenomena such as the quantum, spin and anomalous Hall effect. In contrast to the quantum Hall effect, which is characterized by a global topological invariant and robust against perturbations, the anomalous Hall effect depends on the Berry curvature of occupied bands at the Fermi level and is therefore highly sensitive to subtle changes in the band structure. A unique platform for its manipulation is provided by transition metal oxides, owing to the delicate balance between energy scales and the possibility of creating atomically sharp interfaces, where nanometer-scale electronic and magnetic reconstructions can occur. We demonstrate how electronic transport in the ultrathin ferromagnetic oxide $SrRuO_3$ can be manipulated by imposing asymmetric boundary conditions in the form of two dissimilar interfaces. Measurements of the AHE, which probe the Berry curvature of occupied bands, reveal the presence of two spatially-separated, spin-polarized conduction channels. Using theoretical calculations we show that the Berry curvature of the spin-polarized Ru bands is modified near the $SrTiO_3$ and $SrIrO_3$ interfaces, resulting in opposite signs of the anomalous Hall conductivity. Our study demonstrates how reconstructions at oxide interfaces can be used to control spin and charge accumulation on a nanometer-scale, opening new routes towards spintronics and topological electronics.

Magnetic anisotropy of ferromagnetic oxide thin films studied by angle-dependent XMCD

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Magnetic anisotropy is one of the most important properties of ferromagnetic materials, responsible for the hysteresis of ferromagnets and the perpendicular magnetic anisotropy useful for recording media, and has usually been attributed to the anisotropy of orbital magnetic moment, known as the Bruno model. The model works very well for 3*d* transition metals and their thin films. However, additional contributions from the anisotropic distribution (quadrupole moment) of spin density, represented by the 'magnetic dipole' *T*, may dominate over the effect of the orbital magnetic moment anisotropy.

In order to demonstrate the importance of the anisotropic distribution of spin density, we have measured x-ray magnetic circular dichroism (XMCD) with varying magnetic-field direction. In particular, using 'transverse'-XMCD, where the spin magnetic moment is perpendicular to the incident x-rays, the anisotropic distribution of spin density can be directly measured. As an introduction, results for $L1_0$-ordered FePt thin films, well known for their strong perpendicular magnetic anisotropy, will be presented [1]. Then, we will demonstrate that the magnetic anisotropy of $La_{1-x}Sr_xMnO_3$ thin films, which is sensitive to the epitaxial strain from substrates, can indeed be explained by the anisotropic distribution of spin density induced by the epitaxial strain through spin-orbit coupling [2].

This work has been done in collaboration with M. Kitamura, M. Minohara, K. Yoshimatsu, H. Kumigashira, T. Koide, M. Suzuki, N. Kawamura, T. Seki, K. Takanashi, and A. Tanaka.

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Maximal Rashba-like spin splittings and intrinsic Stoner instabilities at polar surfaces of delafossite oxides

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The ABO_2 family of delafossite oxide metals host a rich array of bulk materials properties, ranging from ultra-high conductivity to unconventional magnetism [1,2]. I will discuss our angle-resolved photoemission (ARPES) studies of the bulk and surface electronic structure of the delafossite oxides (Pd,Pt)CoO_2. I will show how a pronounced self-doping occurrs due to the polar nature of their surfaces. This transforms the system from a single-band non-magnetic nearly-free electron metal in the bulk [3] to an itinerant ferromagnet with strong electron-magnon coupling [4], or to a correlated metal hosting a kinetic-energy-coupled inversion symmetry breaking [5] at their surfaces. The latter maximizes the influence of spin-orbit coupling, allowing this oxide surface to develop some of the largest Rashba-like spin splittings that are known.

Key collaborators on this work include Veronika Sunko (St Andrews and Max-Planck Institute for Chemical Physics of Solids, Dresden), Federico Mazzola (StA), and Helge Rosner, Pallavi Kushwaha, Seunghyum Khim, and Andy Mackenzie (MPI-CPFS).

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Resonant Inelastic X-Ray Scattering on Confined Vanadates and Strained Iridate Films

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Resonant inelastic X-ray scattering (RIXS) is a powerful bulk-sensitive photon-in / photon-out spectroscopic probe of the electronic structure of condensed matter with atomic and orbital sensitivity. It is a unique tool for studying excitations from the electronic ground state in correlated transition-metal oxides, being directly sensitive to lattice-, charge-, orbital- and spin-degrees of freedom. In this talk, we report on a RIXS investigation of the thickness-induced metal-insulator transition in thin films of $CaVO_3$ and a strain manipulation study of the Jeff = ½ state of Sr_2IrO_4.

Controlling transport and magnetic properties in the ultra-thin limit is a prerequisite towards design of more complex heterostructures where emergent phenomena have been widely predicted. Meanwhile, thickness-driven metal-insulator transitions (MITs) in thin films have been reported in recent years in a broad swathe of correlated 3d and 5d transition metal oxides. We report on the evolution of RIXS spectra across the thickness-driven MIT in $CaVO_3$. Bulk $CaVO_3$ is a correlated paramagnetic metal, but with decreasing thickness it evolves towards an insulating state. Our V L_3-RIXS spectra reveal a large transfer of spectral weight from fluorescence to Raman modes and a continuous reduction of electronic bandwidth upon entering the insulating state. Our results suggest that the thickness-driven MIT results from Mott-like correlations that can host charge or spin ordering.

Sr_2IrO_4 has been intensively studied in recent years due to the discovery of a novel J_{eff} = ½ Mott insulating state in the large spin-orbit regime. The sensitivity of this quantum state to local coordination and structural distortions suggests strain and confinement as ideal routes for studying and manipulating its properties. We studied Sr_2IrO_4 thin films, grown on several substrates by pulsed laser deposition, with O K-edge RIXS. The low-energy elementary excitations, encompassing single magnons, bimagnons, particle-hole, as well as spin-orbital excitations, are showing a pronounced dependence on the substrate strain. Our study provides thereby direct evidence that epitaxial strain effectively tunes all the involved energy scales (crystal field, exchange interaction and spin-orbit coupling) which are relevant for the stability of the J_{eff} = ½ state.

Dimensionality-driven metal-insulator-transition in spin-orbit coupled $SrIrO_3$

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Upon reduction of the film thickness we observe a metal-insulator transition in epitaxially stabilized, spin-orbit coupled $SrIrO_3$ ultrathin films [1]. By comparison of the experimental electronic dispersions probed by soft x-ray ARPES with density functional theory at various levels of complexity we identify the leading microscopic mechanisms, i.e., a dimensionality-induced re-adjustment of octahedral rotations, magnetism, and electronic correlations. Our combined spectroscopic and theoretical findings will also be discussed with respect to recent transport experiments on the same system by Groenendijk et al. [2]. The astonishing resemblance of the band structure in the two-dimensional limit to that of bulk Sr_2IrO_4 potentially opens new avenues to unconventional superconductivity by "clean" (i.e., electrostatic) electron doping through field gating of ultrathin $SrIrO_3$.

Work in collaboration with P. Schütz, D. Di Sante, L. Dudy, J. Gabel, M. Stübinger, M. Kamp, G. Sangiovanni, M. Sing (all at U Würzburg), Y. Huang (U Amsterdam), M. Capone (CNR-IOM and SISSA, Trieste), M.-A. Husanu, and V. Strocov (both at Swiss Light Source, PSI).

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Iridates and $RuCl_3$ - from Heisenberg antiferromagnets to potential Kitaev spin-liquids

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The observed richness of topological states on the single-electron level prompts the question what kind of topological phases can develop in more strongly correlated, many-body electron systems. Correlation effects, in particular intra- and inter-orbital electron-electron interactions, are very substantial in 3d transition-metal compounds such as the copper oxides, but the spin-orbit coupling (SOC) is weak. In 5d transition-metal compounds such as iridates, the interesting situation arises that the SOC and Coulomb interactions meet on the same energy scale. The electronic structure of iridates thus depends on a strong competition between the electronic hopping amplitudes, local energy-level splittings, electron-electron interaction strengths, and the SOC of the Ir 5d electrons. The interplay of these ingredients offers the potential to stabilise relatively well-understood states such as a 2D Heisenberg-like antiferromagnet [1,2] in $Sr2IrO_4$, but in principle also far more exotic ones, such a topological Kitaev quantum spin liquid, in (hyper)honeycomb iridates [3-5]. I will discuss the microscopic electronic structures of these iridates, their proximity to idealized Heisenberg and Kitaev models and our contributions to establishing the physical factors that appear to have preempted the realization of quantum spin liquid phases so far and include a discussion on the 4d transition metal chloride $RuCl_3$ [6,7].

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Quantum phenomena in correlated spin-orbit coupled oxide heterostructures

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The controlled synthesis of heterostructures by epitaxial growth to create interfaces between a wide variety of oxide-based quantum materials provides tremendous opportunities for producing materials with remarkable physical properties and functionalities. The strong interfacial orbital hybridization and spin-orbit entangled magnetic interface point to correlated oxide superlattices as an ideal test bed for interface-induced Dzyaloshinskii-Moriya (DM) interactions. Recent studies on oxide heterostructures composed of correlated 3d oxides and spin-orbit coupled 5d oxides have revealed interesting physical properties, which are important to develop oxide-based quantum materials [1-3]. In this talk, we will present our observations on (1) charge transfer induced magnetism and anomalous Hall effect in non-inversion symmetry broken $(SrMnO3)_m(SrIrO_3)_n$ superlattices, (2) the topological Hall effect in inversion symmetry broken $(LaMnO3)_m(SrIrO_3)_n$ heterostructures and its interfacial control, and (3) emergent electronic and magnetic states in 3*d*-5*d* oxide-based double perovskites. The critical role of the DMI and its interfacial control will be discussed together with the potential of 5d TMOs for developing novel quantum informatics.

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Theory of Topological Hall Effect: From Strong to Weak Coupling

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The topological Hall effect (THE) of electrons that arises from the coupling to a noncoplanar spin texture has been studied so far for the strong- and weak-coupling regimes separately; the former in terms of the Berry phase and the latter by perturbation theory. In this work, we present a unified treatment that bridges the strong- and weak-coupling regimes [1]. This is done using the spin gauge field, by considering not only the adiabatic (Berry phase) component of the gauge field but also the nonadiabatic component. While only the adiabatic contribution is important in the strong-coupling regime, it is completely canceled by the nonadiabatic contribution in the weak-coupling regime, where the THE is governed by the remaining nonadiabatic terms. We found a new weak-coupling region that cannot be accessed by a simple perturbation theory, where the Hall conductivity is proportional to the exchange splitting of the electron spectrum. The result seems to offer a good explanation for the very large THE found recently in Ce-doped $CaMnO_3$ thin films [2].

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Exotic spin-orbital entangled states in 4d and 5d complex oxides

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Recently, 4d and 5d transition metal oxides (TMO) emerged as a new paradigm in strongly correlated electron research, where strong spin-orbit coupling meets with electron correlations. Using perovskite related 4d- and 5d- complex oxides with t2g electrons, we show that the strong spin-orbit coupling, and the resultant spin-orbital entangled j moments, can give rise to unusual “non-magnetic” Mott insulators and exotic magnets such as a topological quantum spin liquid where anisotropic. The topics will include the following.

(I) $5d^5$ j_{eff} = 1/2 spin-orbital quantum liquid on honeycomb lattice in $H_3LiIr_2O_6$ [1], reminiscent of the Kitaev model.

(II) $4d^4$ J_{eff} = 0 Mott insulator [2] in Ru^{4+} oxides, proximity to excitonic magnetism.

(III) $5d^1$ multipolar ordering of j_{eff} = 3/2 in the absence of magnetic dipole moment in double perovskite-like Ta^{4+} chlorides [3].

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Spinorbitronics in engineered $SrTiO_3$-based 2-dimensional electron systems

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Despite being a wide bandgap insulator, $SrTiO_3$ (STO) is a very interesting oxide template to form 2-dimensional electron systems (2DES). The first STO-based 2DES was discovered at the interface with another wide bandgap insulator, LaAlO3 (LAO) [1], but it was later found that STO surfaces could also become metallic in vacuum [2] and that a 2DES would form if a reactive metal such as Al was deposited onto STO [3]. STO-based 2DES possess common features, such as typical carrier densities in the 10^{13} cm^{-3} range, splitted Ti 3d bands with different orbital character, a strong sensitivity to electrostatic effects and gating, and relatively long scattering times. In addition, the electric field present in the 2DES region results in a Rashba effect that is sensitive to a gate voltage [4].
In this talk, we will show how the electronic properties of LAO/STO 2DES can be tuned by depositing different metallic overlayers [5].
We will then make use of the Rashba effect in the 2DES to achieve spin-charge conversion (SCC). Through spin-pumping, we inject a spin current from a ferromagnetic film into the oxide 2DES and detect the resulting charge current. The SCC can be strongly modulated by a gate voltage, in amplitude and sign [6]. We will discuss this gate dependence on the basis of the electronic structure of the 2DES.

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Oxide heterostructure based magneto-transports

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The broken inversion symmetry at the $LaAlO_3/SrTiO_3$ (LAO/STO) interface results in the presence of a Rashba spin-orbit (SO) field. The simultaneous existence of ferromagnetism and tunable Rashba SO coupling (SOC) in LAO/STO allows the use of magneto-transport studies to probe the SO fields at the LAO/STO interface. We experimentally showed that anisotropic magnetoresistance (AMR) can be used as a powerful tool to study both magnetic ordering as well as the Rashba field of 0.17 T at a current density of 10^8 A/m^2 in LAO/STO [1].

In addition, an angular dependent study of MR measurements in LAO/STO revealed the existence of a new type of MR that is similar to the spin Hall MR. Due to the interfacial nature of a LAO/STO 2DEG, the observed phenomenon can be called the interfacial Rashba MR [2]. The magnitude of interfacial Rashba MRs in LAO/STO (~7%) is much larger than the reported spin Hall MR of ferromagnet/heavy metal structures (0.01 − 1%).

One practical application of this strong Rashba SOC in the LAO/STO in spintronics is to convert a charge current into spin current that can be used to control the magnetization of an adjacent FM using spin-orbit torques (SOTs). We demonstrated a giant room temperature charge-to-spin conversion efficiency of 6.3 in the STO/LAO/CoFeB structure [3], which is almost 2 orders of magnitude larger than the spin Hall angles in conventional heavy metals.

Finally, we examine the role of oxygen bonding in Pt/CoFeB by changing the thickness of the SiO_2 capping layer. We find that as the oxygen bonding level in CoFeB increases, not only a magnitude change but also a full sign reversal of SOTs occur [4]. While the magnitude change can be explained within the bulk spin Hall model, the full sign reversal goes beyond the bulk spin Hall effect and evidences an interfacial SOT mechanism such as the Rashba effect. We estimate that the new mechanism in our sample can be two times stronger than the bulk spin Hall mechanism.

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Emergent functionalities at oxide heterointerfaces induced by spin orbit interactions

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Breaking of inversion symmetry at perovskite surfaces and its stabilization at heterointerfaces lead to emergent functionalities that are not present in bulk. When combined with spin-orbit interactions this enables new mechanisms to control spin states and new device applications ranging from electric field control of electronic devices, voltage control of magnetic state as well new spin textures. The material platforms that will be discussed in this talk are based on oxide semiconductors of doped $SrTiO_3$ coupled with spin injection interfaces comprising of 3d transition metals and other complex oxides. The talk will illustrate how the interfaces of such simple spintronic devices enable the tuning of electronic and spin transport parameters by coupling the intrinsic electric fields with Rashba spin orbit fields. The ability to create, and control new phenomena in such devices is important for fundamental research that drives new technologies and upcoming architectures.

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Oxygen vacancy controlled functionalities in multiferroic tunnel junctions

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Oxygen vacancies are the most common defect in perovskite oxides. Important applications are associated with their controlled generation and transport in electrochemical energy and memory devices. In nanostructures oxygen vacancies can accumulate under the action of external electric fields and be the source of novel functionalities. Here, we make use of the dynamic control of the vacancy profile in the nanometer thick barrier of a ferroelectric tunnel junction to demonstrate the interplay between resistive (oxygen vacancy) and ferroelectric switching. Oxygen vacancies generated in an electrochemically active ferroelectric barrier control the stability of the ferroelectric polarization and modify its coercive fields. Further, I will show that oxygen vacancies stabilize unexpected domain structures in the ferroelectric barrier which control the tunneling transport providing a major step forward towards the new concept "The Wall is the Device" [1]. The strong coupling between electrochemical and electronic degrees of freedom sheds light on the growing debate between resistive and ferroelectric switching in multiferroic tunnel junctions, and can, moreover, be the source of novel concepts in memory devices and neuromorphic computing.

Work done in collaboration with J. Tornos[1], G. Sanchez-Santolino[2], D. Hernandez-Martin[1], F. Gallego[1], G. Orfila[1], M. Cabero[1], A. Perez-Muñoz[1], J. I. Beltran[1], C. Munuera[2], A. Rivera-Calzada[1], Z. Sefrioui[1], F. Mompean[2], M. Garcia-Hernandez[2], S. J. Pennycook[3] , M. Varela[1], M. C. Muñoz[2], S. Valencia[4], Y. H. Liu[5,6], V. Lauter[5], R. Abrudan[4], C. Luo[4], R. Hanjo[4], F. Radu[4] Q. Wang[6], S. G. E. te Velthuis[6], C. Leon[1],

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Charge and spin transitions in perovskite-structure oxides containing unusually high-valence Fe

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Charge and spin transitions in transition-metal oxides are topics of interest in fundamental solid-state chemistry and condensed matter physics. The charge transition behaviors highlight the electronic instability of these materials and give information on charge-spin-lattice couplings in the system. In a few oxides containing unusually high-valence Fe, such electronic instabilities are relieved by distinct charge transitions; charge disproportionation as seen in $CaCu_3Fe_4O_{12}$ ($4Fe^{4+} \rightarrow 2Fe^{3+} + 2Fe^{5+}$) and intermetallic charge transfer as seen in $LaCu_3Fe_4O_{12}$ ($3Cu^{2+} + 4Fe^{3.75+} \rightarrow 3Cu^{3+} + 4Fe^{3+}$), both of which are accompanied by spin transitions [1]. Recently successive charge transitions, the charge disproportionation and then the intermetallic charge transfer, of $Fe^{3.5+}$ were found in $Ca_{0.5}Bi_{0.5}FeO_3$ [2]. Both transitions are also associated with unusual structural and magnetic changes [3]. The transition behavior is in contrast to the single charge disproportionation transition of $Fe^{3.5+}$ in $Sr_{0.5}Bi_{0.5}FeO_3$ [4]. The unusual charge and spin transitions of the newly discovered compounds are described and the charge-spin-lattice couplings of the system are discussed.

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Functional Properties of $CaFeO_3$ and $SrFeO_3$ Heterostructures

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Ferrate perovskites that contain the unusually high Fe^{4+} oxidation state, such as $CaFeO_3$ and $SrFeO_3$, host a collection of novel physical properties including coupled structural and electronic phase transitions, helical magnetism, and negative charge transfer physics. The ability to make heterostructures of these materials enables studies of how these phenomena can be altered or tuned through epitaxial strain, interfacial formation, and finite thickness effects. We have synthesized $CaFeO_3$ and $SrFeO_3$-based heterostructures using oxygen plasma-assisted molecular beam epitaxy. Transport measurements of strained $CaFeO_3$ films reveal that its metal-insulator transition temperature is suppressed under both compressive and tensile strain. Performing X-ray spectroscopy measurements across the $CaFeO_3$ metal-insulator transition, we find clear changes to the oxygen-derived electronic structure, but not to the iron-derived states, consistent with a bond disproportionation model in which oxygen ligand holes play a central role in the electronic phase transition.[1] Results will also be presented on the magnetic properties of ferrate heterostructures including magnetotransport and resonant scattering experiments that confirm the presence of helical magnetism in the heterostructures.

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Ferroelectrically tunable magnetic skyrmions in ultrathin oxide heterostructures

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Magnetic skyrmions are topologically protected, whirling spin texture in nanoscale.[1] Its small size, topologically-protected stability, and solitonic characteristics together hold great promises for future spintronics applications.[2] To translate such compelling features into practical spintronic devices, a key challenge lies in achieving effective controls of skyrmion size, density, and thermodynamic stability. Here, we report the discovery of ferroelectrically tunable skyrmions in ultrathin $BaTiO_3/SrRuO_3$ bilayer heterostructures.[3,4] The ferroelectric proximity effect at the $BaTiO_3/SrRuO_3$ heterointerface can trigger a sizable Dzyaloshinskii-Moriya interaction, thus stabilizing robust high-density skyrmions. The minimum skyrmion size in this system can reach approximately 10 nm. Moreover, by manipulating the ferroelectric polarization of $BaTiO_3$, we achieve local, switchable and nonvolatile tunability of both skyrmion density and thermodynamic stability. Such ferroelectric control of skyrmion properties heralds a novel approach toward improvements in the integratability and addressability of skyrmion-based functional devices.

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Magnetoelectric multi-spin variables in complex transition-metal oxides

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One of the most important concepts in condensed matter physics is the spontaneous breakdown of symmetry in a solid, which bears the ordered phase and domains in its consequence. In multiferroics having two or more ferroic orders simultaneously, multiple order parameters coexist in a system, sometimes couple with each other, and exhibit nontrivial crossed phenomena such as magnetoelectric effect. In this study, we deal with multi-spin variables which break both the time reversal and the space inversion and result in magnetoelectric activity as well as nonreciprocal wave propagation. Examples of such variables are magnetic toroidal and magnetic quadrupole moments. We introduce our strategy of how to embed such variables in complex transition-metal oxides and show our recent achievements for the experimental demonstrations.

This work was done in collaboration with K. Kimura (U. Tokyo), H. Ueda (Osaka U.), Y. Yamaguchi (Osaka U.), Y. Araya (Osaka U.), R. Misawa (U. Tokyo), T. Katsuyoshi (U. Tokyo), Y. Tanaka (RIKEN), S. Kimura (Tohoku U.), and Y. Sawada (Osaka U.).

Polar metals, ferroelectric metals

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Can a metal present a polar distortion that breaks the inversion symmetry of the lattice? (In spite of the fact that the usual driving force for ferroelectricity are Coulomb dipole-dipole interactions that all but vanish in metals.) If so, would we be able to switch such a polar distortion with an external bias? (Despite the fact that metals are not supposed to sustain voltage drops.) The interest in these questions is many-fold, from fundamental to applied. Indeed, it is always good to understand what's possible and what's not; besides, non-centrosymmetric (polar) metals are rare creatures (certainly among perovskite oxides) potentially useful in various contexts. With a number of collaborators – most notably H.J. Zhao (LIST), and A. Filippetti and V. Fiorentini (Cagliari) –, we have studied these problems using first-principles simulations and have run into a few discoveries in the way. We have found that the answer to the first question is an affirmative one; as a matter of fact, we have identified a previously unnoticed, seemingly-universal "meta-screening" effect that favors polar order in metallized ferroelectrics [1]. As for the second question, we are now convinced that, in well-chosen conditions, it is possible to apply an external electric field to a metal and switch its polar distortion, which yields a genuine *ferroelectric metal*! [2] As a result, we think we have access to a new and fairly exciting family of materials that are likely to surprise us with additional unexpected behaviors. In this talk I will summarize these works.

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Ferroic Domain Walls for Transient Nanoelectronics and Phononics

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It is now well-established that ferroelectric domain walls can act as pseudo-two dimensional (2D) electrical conductors [1]. Sometimes conduction appears to be metallic [2] but, more often than not, semiconducting properties are observed. Both p and n-type carriers may be active, depending on the nature of the domain wall polarization discontinuity [3]. If p and n-type domain walls meet (reasonably common in certain microstructures), a 1D line p-n junction is expected. Since domain walls can be moved around or be made to disappear, such 1D p-n diodes (and hence potentially transistors) should be both mobile and ephemeral in nature: "now-you-see-it, now-you-don't". However, investigations into the existence, electrical properties and potential transience of these domain wall p-n junctions are at a very early stage. This talk will describe recent progress in mapping Hall voltages [4] generated by active carriers in conducting domain walls in $ErMnO_3$, using Kelvin Probe Force Microscopy (KPFM). Analysis reveals the carrier type, number density and mobility in both head-to-head and tail-to-tail walls and confirms that vertex domain wall junctions are points at which current-carrying n- and p-type domain walls meet.

In a separate study, the phonon scattering behaviour of ferroelastic domain walls in $LaAlO_3$ has been examined through mapping the bulk thermal conductivity as a function of temperature. Strong domain wall-related scattering is observed at low temperatures. This suggests that transient domain microstructures could be used to actively control phononic pathways in the future.

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Tuning functional properties of $BiFeO_3$ films using strain and growth chemistry

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Multiferroics – materials with coexisting ferroic orders such as ferroelectricity and (anti)-ferromagnetism – are presently under intense study by virtue of their promise in next-generation data storage devices. Bismuth ferrite ($BiFeO_3$ – BFO) is one of the very few that orders above room temperature. In the bulk, BFO is rhombohedral (R), and in thin films [1] its properties are sensitive to strain [2,3]. The discovery of the epitaxially-stabilized "super tetragonal phase" of BFO (T-BFO) [4] incited a flurry of research activity focused on understanding the phase transition and its possible functionalities [5]. T-BFO is also multiferroic, with large ferroelectric polarization and antiferromagnetic order [4], and the strain relaxation-induced T/R phase mixtures and their exceptional piezoelectric responses [6] continue to intrigue and motivate researchers. A particularly important characteristic of this phase mixture is the interconversion between the R,T phases with an applied electric field [6]. Since the oxygen configuration of the R and T polymorphs is different [5], the electronic, magnetic, and optical properties can thus be dynamically modulated. An additional rather crucial aspect of mixed R/T BFO is the role of *chemistry* in the formation of the metastable T-phase. Since T-BFO is typically fabricated by pulsed laser deposition, growth parameters can be used as a strong handle to tailor film properties and functionalities.

Here we describe the influence of strain and growth conditions on the optical, magnetic, and ferroelectric properties of BFO films. We also show that by precisely controlling the fabrication conditions, the formation of the mixed R/T phase can be completely suppressed for film thicknesses up to 100 nm. Such a result is useful for applications where thicker pure T-BFO films are needed, such as for measuring the giant polarization, or for precisely controlling the proportions of the various phases. Finally, through analysis of a large set of epitaxial films, we show that the optical band gap of BFO is rather insensitive to a host of growth and processing parameters [7]. Combined with the numerous other functionalities of this material, one can envisage multifunctional devices, for example, that harvest mechanical and solar energy, or to enhance magnetoelectric coupling at these phase boundaries.

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Uncovering switching and failure mechanism in memristive devices by *operando* spectromicroscopy

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It is suspected that voltage-driven oxygen-ion migration and the resulting nanoscale redox processes drive the resistance change in transition metal oxide based memristive devices. Direct observation of the switching and failure mechanism, however, remain challenging because the net changes of structure, stoichiometry, and valence state during switching are very small and occur primarily at electrode interfaces or within nanoscale filaments.

Here we will present local changes in the chemical and electronic structure of $SrTiO_3$-based memristive devices utilizing high-resolution *operando* characterization tools like transmission electron microscopy (TEM) [1] and photoemission electron microscopy (PEEM) [2,3]. We chose $SrTiO_3$ as a single crystalline model material, which offers a well-understood platform and well-characterized spectroscopic signatures.

To overcome the surface sensitivity typically limiting PEEM investigations of memristive devices, photoelectron-transparent graphene top electrodes were used to attain spectroscopic information from the buried $SrTiO_3$ layer [1]. Quantitative maps of the oxygen vacancy concentration obtained during *in situ* switching confirm that localized oxygen evolution and reincorporation reactions rather than purely internal movement of oxygen vacancies cause the resistance change [1].

Comparison of devices with intrinsically different levels of data retention showed that all $SrTiO_3$-devices with a stable retention exhibit a local phase separation within the switching filament consisting of a SrO overlayer on a Sr-deficient $SrTiO_3$. This SrO overlayer provides a diffusion-blocking layer which is a necessary component for long data retention times. Intentional incorporation of layers with slow oxygen diffusion therefore constitutes a design rule for retention-failure-resistant devices [2].

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Enhanced lithium transport in highly ordered complex oxide cathode films towards solid-state batteries

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Solid-state microbatteries can facilitate miniaturization, create more flexibility for the design of stand-alone microelectronic devices and enhance their applicability, for example in medical implants, due to the avoided leakage risks. However, the successful application of all-solid-state microbatteries depends strongly on the enhancement of energy density and lifetime. The cycle-life and lifetime are dependent on the nature of the interfaces between the electrodes and electrolyte, whereas safety is a function of the stability of the electrode materials and interfaces. Therefore, perfect control on the interfacial properties between the electrodes and electrolyte is needed, but remains a great challenge.

Various oxide materials are known as promising cathode materials as they provide good thermochemical stability, high energy density and high voltage. However, the crystal structure of the main candidates (spinel $LiMn_2O_4$, layered $LiCoO_2$ and olivine $LiFePO_4$) exhibit distinct differences in the lithium diffusion behavior along 3D, 2D and 1D directions respectively. Common bulk studies on battery materials investigate polycrystalline films and, therefore, do not enable detailed characterization of the ionic and electrical conductivity along specific crystalline orientations. Furthermore, the formation of the unwanted solid electrode interphase (SEI) layer between a cathode and electrolyte varies strongly depending on the specific crystal facet of the cathode material. Single crystalline thin films of cathode materials are required to obtain more insight into the ideal interface ordering and the corresponding ionic and electrical properties.

Here, we will show the lithium diffusion behavior in $LiMn_2O_4$ cathode (and $Li_4Ti_5O_{12}$ anode) thin films, which are epitaxially grown by pulsed laser deposition on single crystalline Nb-doped $SrTiO_3$ substrates. Control over the specific crystal orientation of the full thin film enables detailed analysis of the lithium diffusion along specific crystal planes ({001}, {110} and {111}). Single phase films show enhanced cyclability and faster charging speed, as compared to studies on polycrystalline materials. The achieved capacity reached >90% of the theoretical limit and minimal capacity reduction was observed when measured over 1000 cycles. High charge-discharge speeds in the range 1C-30C showed good capacity retention.

Highly Stable Artificial STDP Synapse Based on Oxide FET

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Artificial neural networks (NNs) have recently attracted much attention by demonstrating their potential for implementing human-like intelligent processing. Nowadays, most of the NN computing systems consist of a huge number of Si-based CMOS and their high-power consumption is a critical issue for developing much larger systems. To solve this issue, chips specialized for NN computing, called neuromorphic chips, have been developing by using emerging devices. One of the essential elements of neuromorphic chips is an artificial synapse, and most of the present artificial synapses are based on two-terminal resistive switching (RS) memories such as memristors and phase-change memories. These RS-memory-based synapses utilize stochastic events such as a filament formation and thus the instability on voltage pulses is inevitable. For deep NN computing such as convolutional NN computing, however, a stable artificial synapse is demanded.

In this study, we have developed a highly-stable spike-timing-dependent plasticity (STDP) synapse based on an oxide field-effect transistor (FET) consisting of $SrTiO_3$ (STO) channel [1]. The STO FET presents a gate-controlled insulator-to-metal transition (IMT), if the gate voltage V_{GS} is above $V_{IMT} \sim 3.5$ V. After the IMT, the STO FET shows a substantial hysteresis in the drain current I_D–V_{GS} characteristics, a key element of synaptic functionalities. In contrast to conventional RS-memory-based synapses, our STDP synapse shows a distinguished stability with a large dynamic range, due to the nature of the metallic channel of the STO FET. We also demonstrated handwritten digits recognition in a simulated spiking neural network (SNN) for our STDP synapse and unravelled that a nonlinearity of the threshold shift against the gate voltage is the essential property for STDP.

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Imaging, controlling and harnessing non-collinear magnetism in perovskite oxides

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In magnetic perovskite oxides ABO_3, first-neighbour antiferromagnetic super-exchange interactions usually dominate, but may coexist with other terms such as ferromagnetic double-exchange or Dzyaloshinskii-Moriya interactions at B-O-B and A-O-A bonds. This often produces non-collinear spin configurations leading to weak ferromagnetism or to spatially modulated spin structures. A prototypical non-collinear magnetic oxide is multiferroic $BiFeO_3$ that shows a cycloidal order with a 64 nm period in the bulk [1]. In this talk, I will show how epitaxial strain can be used to tailor the magnetic order of $BiFeO_3$ thin films [2,3] and present real-space images of the cycloidal structure, as well as its manipulation by an electric field [4]. In a second part, I will report the observation of a very large topological Hall effect (THE) in thin films of a lightly electron-doped manganite. Magnetic force microscopy reveals the presence of small magnetic bubbles, whose density vs. magnetic field peaks near the THE maximum, as is expected to occur in skyrmion systems. The THE critically depends on carrier concentration and diverges at low doping, near the metal-insulator transition. I will discuss this observation of a THE in a weak-coupling regime with non-adiabatic contributions [5] beyond the conventional picture, and the strong amplification of this topological phenomenon by correlation effects.

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Electronic transport and microscopic imaging in magnetic interfaces

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In the first part of the talk I will discuss the spatial extent of electronic reconstruction emerging at oxide interfaces such as in $LaAlO_3/SrTiO_3$: we identify narrow 2D interfaces housing superconductivity and/or other emergent phases, electronically isotropic regions far from the interface, and intermediate zones where interfacial proximity renormalizes the electronic structure relative to the bulk. Furthermore, a hysteretic in-plane magnetoresistance develops below the superconducting transition possibly from vortex depinning within a thin superconducting layer, in which the vortices are created by discrete ferromagnetic dipoles located solely above the layer.

In the second part I will focus on the topological Hall transport in magnetic materials due to chiral interactions. Using materials hosting particle-like spin structures as a paradigm, I will demonstrate direct correspondence between magnetic skyrmions and their topological Hall signature by combining transport and magnetic force microscopy measurements over a wide range of temperature and magnetic field. We identify a much larger topological Hall resistivity than prevailing theory predicts and address the implications for the impact of the Berry-phase on charge carriers.

Electronic and optical properties of rare earth titanates

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The rare-earth titanates ($RTiO_3$, where R is a rare-earth atom) have become the focus of great interest because of their use in complex-oxide heterostructures that display two-dimensional electron gases (2DEGs) with unprecedented high densities [1,2]. These compounds are Mott insulators, with a Mott-Hubbard gap opening up within the Ti 3*d* states. This gap is commonly reported to be 0.2-0.7 eV across the series, based on the onset of optical absorption. We demonstrate that the Mott-Hubbard gap of GTO is actually much larger, close to 2 eV. This conclusion is based on both first-principles calculations (using hybrid density functional theory) and photoluminescence (PL) measurements [3].

The experimentally observed onset in absorption is not related to the gap, but is associated with small polarons [4]. We have also performed a study of other impurities and point defects that may affect the conductivity [5]. Among native defects, the cation vacancies have the lowest formation energies in oxygen-rich conditions, and oxygen vacancies have the lowest formation energy in oxygen-poor conditions. Among the impurities, Sr_{Gd}, H_i and C_O are easily incorporated. The defects and impurities are intrinsically stable only in a single "natural" charge state, to which various numbers of hole polarons can be bound, which explains the frequent observation of *p*-type hopping conductivity in the rare-earth titanates.

Given the similarities in electronic structure between the rare-earth titanates, our results for GTO have repercussions for the other members of the series. The results also affect the design of complex-oxide heterostructures involving these materials.

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Charge Transfers Across Oxide Interfaces Hosting a 2-Dimensional Electron Gas

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The origin of the carriers populating the 2-Dimensional Electron Gas (2DEG) found at the $LaAlO_3/SrTiO_3$ and similar interfaces is still controversial. While a number of individual experiments seem to correlate the 2DEG formation with specific material properties, as $LaAlO_3$ polarity or oxygen vacancy formation, a model able to show a predictive power and to account for the conductivity of different oxide interfaces, having either a crystalline or an amorphous overlayer, is still missing. In this talk, the conducting properties of the amorphous-$LaAlO_3/BaTiO_3/SrTiO_3$ heterostructure will be presented and a number of experiments on amorphous, crystalline and hybrid conducting interfaces will be described. The constraints set by these experiments on the possible applicable mechanisms will be shown and discussed.

Square-lattice TMO monolayers and Van der Waals heterostructures

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Most two-dimensional materials, e.g., graphene, transition-metal dichalcogenides, etc., have a hexagonal lattice. In their bulk form, transition-metal oxides are typically cubic. Here we describe joint theoretical experimental work (see collaborators in the lists of co-authors [1,2]) in two cases where square-lattice TMO monolayers have been fabricated and studied, exhibiting interesting properties. The first case [1] is the formation of copper oxide monolayers on a graphene substrate or within graphene nanopores. A synergistic application of density-functional-theory (DFT) calculations and experimental measurements establishes the stoichiometry of the oxide as CuO. The monolayers are predicted to have interesting electronic and magnetic properties. In the second case [2], we first use DFT calculations to show that a recently observed VO_2 monolayer that serves as an interlayer in the growth of bronze-phase VO_2 on TiO_2 [3] is bonded by van der Waals interactions. We then use new scanning-transmission-electron-microscopy (STEM) images of monolayer FeSe on $SrTiO_3$ and corresponding DFT calculations to identify the structure of an interfacial square-lattice Ti-O interlayer and demonstrate that it has a $Ti_{1.5}O_2$ composition and is also bonded by van der Waals interactions [3]. Further calculations [3] demonstrate that this monolayer plays a crucial role in explaining the observed [4] enhancement of the critical temperature of the superconductivity in the FeSe monolayer an order of magnitude higher than its value in bulk FeSe.

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