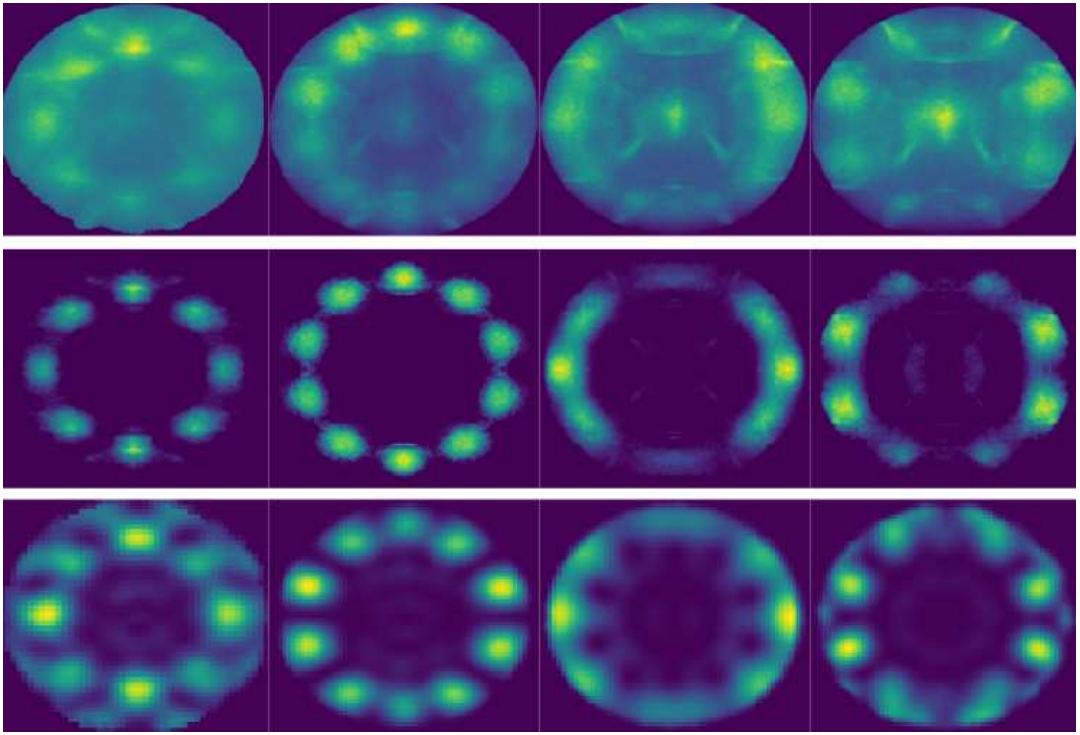
Condensed Matter Physics



Condensed matter theory

Prof. Titus Neupert

We study **topological phases of quantum matter** with numerical and analytical tools. Topological electronic states are characterized universal and robust phenomena, such as the Hall conductivity in the integer quantum Hall effect, that are of fundamental interest or promise applications in future electronics. We study and propose **concrete materials** to realize such topological effects, but are also interested in studying abstract models to understand what phases of matter can exist in principle.
Our numerical toolbox includes **neural network algorithms** to study strongly interacting quantum many-body systems. Furthermore, we work at the interface of **quantum computing** and condensed matter physics.

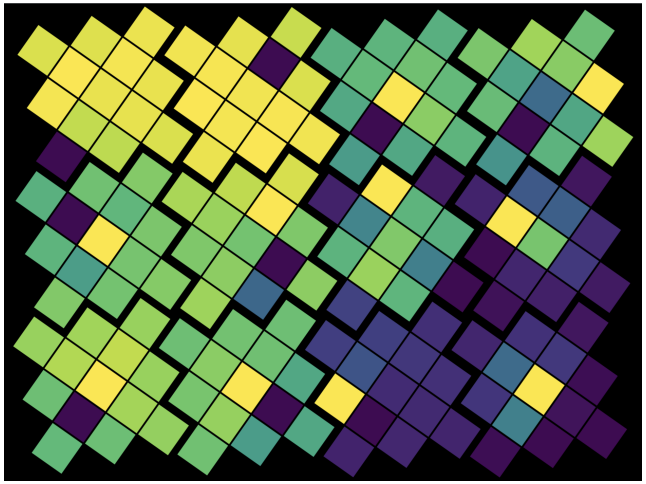
https://www.physik.uzh.ch/g/neupert

Machine learning meets condensed matter physics

Deep learning is everywhere in science and technology. Recently, it also starts to enjoy applications in quantum matter research. In 2019, a growing number of activities in our group were focused on these artificial intelligence techniques.

Most immediate is the use of neural networks to analyze various forms of experimental data or to aid experiments. As an example, Pascal Vecsei studied in his bachelor thesis how machine learning can be used to deduce the space group of a crystal based on powder x-ray diffraction curves. This is a challenging task which usually takes the experience of a crystallographer. We used a neural network for the classification of the crystal structures into one of the 230 space groups of nonmagnetic materials with the help of theoretically computed test data. When used on real data of rather low quality, the algorithm identified the correct space group more than half of the time. If the algorithm is also allowed to flag bad datasets, its accuracy on the good ones goes up to 80%.

A completely different application of machine learning is explored by the group members Kenny Choo and Nikita Astrakhantsev, who use neural networks as compressed representations of complex many-body wave functions. The underlying problem is that even for relatively small



Neural networks can be used efficiently as a compressed representation of complex quantum many-body states, that could otherwise not be stored on any computer memory. Shown is a color scale representation of some of the weights of a neural network quantum state that approximates to high accuracy the ground state of the Heisenberg model on the square lattice.

quantum many-body systems it is not possible to store the exact quantum state in any available computer memory. One has to resort to compressed representations, and neural networks provide an opportunity for this. In a collaboration led by the Flatiron Institute in New York, Kenny Choo co-developed a software package called Netket (www.netket.org) that allows to perform computations with these neural network quantum states. We applied this new methodology to the J1-J2 spin-1/2 Heisenberg model on the square lattice, a classic frustrated problem in quantum magnetism. We found that the neural network quantum states outperform other techniques almost everywhere in the phase diagram. Going forward, we want to employ this new methodology to solve very challenging quantum many-body problems, such as three-dimensional frustrated magnets.

Alongside these research activities, we also co-organized a symposium entitled "Artificial Intelligence and the Scientific Method" in September 2019, which brought together high-profile scientist from a diverse set of fields that use machine learning for their research.

Highlighted Publications:

1. Neural network based classification of crystal symmetries from x-ray diffraction patterns,
   Vecsei, P.M. *et al.*, Phys. Rev. B **99**, 245120 (2019)
2. NetKet: A machine learning toolkit for many-body quantum systems,
   Carleo, G., *et al.*, SoftwareX **10**, 100311 (2019)
3. Study of the Two-Dimensional Frustrated J1-J2 Model with Neural Network Quantum States,
   Kenny Choo, *et al.*, Phys. Rev. B **100**, 125124 (2019)

Superconductivity and Magnetism

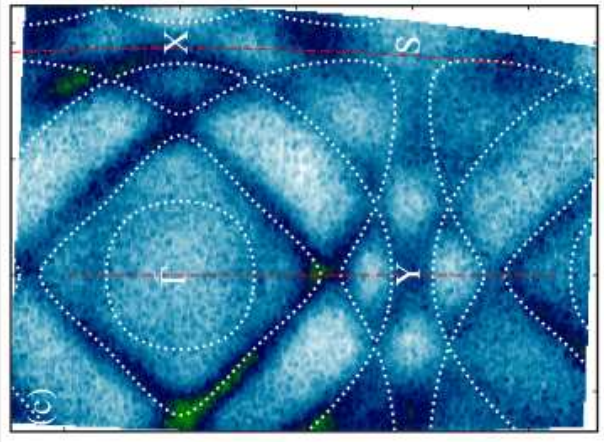
Prof. Johan Chang

We investigate **quantum matter phases emerging from strong electronic interactions**. High-temperature superconductivity, strange metals, density-wave instabilities and electronic driven metal-insulator transitions are studied by synchrotron and laboratory based experimental techniques. At international synchrotrons, we are carrying out angle-resolved photo-emission spectroscopy (ARPES) and resonant inelastic x-ray scattering (RIXS) to reveal electronic structures and properties of correlated electron systems. Quantum phase transitions tuned by magnetic field or hydrostatic pressure are furthermore explored by high-energy x-ray diffraction. Within our laboratory, similar themes are probed by electrical and thermo-electrical transport measurements. Our group also has technical initiatives to develop innovative and compact cryo-cooling methodology. Finally, we are involved in single crystal synthesis through interdisciplinary collaborations with solid state chemists.

https://www.physik.uzh.ch/g/chang

Orbitally selective Fermi liquid breakdown.

Correlated metals are typically classified either as Fermi liquids or non-Fermi liquids depending on whether or not resistivity scales with temperature squared. There is, however, transport evidence suggesting that some materials are hybrids of these two metal classes. This mixed regime is of particular interest as it provides insight into how Fermi liquids break down and the nature of non-Fermi-liquid quasiparticles. In this context, multiorbital metallic systems in conjunction with strong Hund's coupling and electron correlations are of great conceptual importance. Using photoemission spectroscopy, we demonstrated that $Ca_{1.8}Sr_{0.2}RuO_4$ is neither a standard Hunds metal nor representing orbital-selective Mott physics. In fact, the thermally excited state constitutes an example of a hybrid metal.



Fermi surface of $Ca_{1.8}Sr_{0.2}RuO_4$ recorded using angle resolved photoemission spectroscopy.

Parental control of Mott-insulating La_2CuO_4.

An outstanding challenge in high-temperature superconductivity is to understand the optimal conditions for superconductivity: which microscopic parameters drive the change in T_c and how can we tune them? We demonstrated, by a combination of x-ray absorption and resonant inelastic x-ray scattering spectroscopy, how the Coulomb and magnetic-exchange interaction of La_2CuO_4 thin films can be enhanced by compressive strain. Our experiments and theoretical calculations establish that the substrate producing the largest T_c under doping also generates the largest nearest-neighbour hopping integral, Coulomb and magnetic-exchange interaction. We hence suggest optimising the parent Mott state as a strategy for enhancing the superconducting transition temperature in cuprates.

Highlighted Publications:

1. Strain-engineering Mott-insulating La_2CuO_4, O. Ivashko *et al.*, Nature Communications **10**, 786 (2019)
2. Orbitally selective breakdown of Fermi liquid quasiparticles in $Ca_{1.8}Sr_{0.2}RuO_4$, D. Sutter *et al.*, Physical Review B **99**, 121115(R) (2019)
3. Band structure of overdoped cuprate superconductors: Density functional theory matching experiments, K. P. Kramer *et al.*, Physical Review B **99**, 224509 (2019)

Oxide Interface Physics

Prof. Marta Gibert

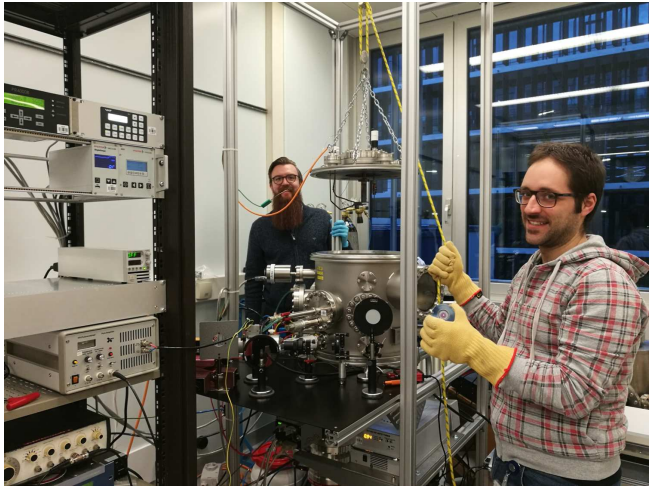
Complex-oxide heterostructures, consisting of layers of different oxide compounds stacked one on top of another with atomic precision, are of interest because the many routes they offer for the manipulation of the physical properties of these materials and the engineering of novel functionalities. Reduced dimensionalities and structural and electronic couplings originating at the interfaces have led to some of the most interesting findings.

In our group, we focus on the study of interface physics phenomena in complex oxides. Our research encompasses from the growth of high quality oxide heterostructures to the detailed study of their structural and electronic properties, both in the laboratory and also in large scale facilities.

https://www.physik.uzh.ch/g/gibert

Transition metal oxides (TMOs) are an extensive class of compounds displaying a large variety of interesting physical properties (i.e. metal-insulator transitions, magnetism, multiferroicity, superconductivity, etc.), which makes them highly attractive candidates for next-generation electronic devices. All these functionalities stem from strong electronic correlations and a complex interplay between the charge, orbital, spin and lattice degrees of freedom. These compounds often crystallize in rather similar crystalline structures enabling the generation of artificially layered structures (i.e. thin films, superlattices) as a means to tailor their properties. In our group, we grow high-quality oxide heterostructures by off-axis radiofrequency magnetron sputtering.

During the last year, our research has mainly focused on the family of double-perovskite compounds A_2NiMnO_6 (A being a rare earth cation), which is characterized by an insulating ferromagnetic behaviour. Ferromagnetism is often accompanied by metallicity, and thus ferromagnetic insulators are scarce compounds but of high interest in fields such



Jonathan Spring and Gabriele De Luca growing a La_2NiMnO_6 thin film by off-axis rf magnetron sputtering.

as spintronics. We have been extensively studying the end member La_2NiMnO_6, which displays high Curie temperature (T_c∼280K). A rock-salt arrangement of the corner-sharing NiO_6 and MnO_6 building blocks of the double-perovskite structure is key for such magnetic behaviour. A variety of tools (x-ray diffraction, atomic force microscopy (AFM), SQUID-magnetometry, x-ray absorption spectroscopy (XAS), transmission electron microscopy (TEM), etc.) has been used to prove the long-range order of the Ni^{2+} and Mn^{4+} cations and to show that the bulk-like magnetic properties are achieved in our thin films.

The magnetism of the La_2NiMnO_6 films has been investigated as function of the epitaxial strain by synthesizing the layers on different substrates and as function of thickness by growing films down to only few unit cells (u.c). La_2NiMnO_6 films as thin as 2 nm (5 u.c.) are found to still exhibit a ferromagnetic behaviour with T_c∼200K. We are now investigating the origin of such thickness-driven reduction of the magnetic properties in order to overcome it. To that aim, special emphasis is given to understand the role of interfacial phenomena (strain, coupling of oxygen octahedral rotations, polar discontinuity, etc.) in ultrathin epitaxial La_2NiMnO_6 layers.

Low dimensional systems

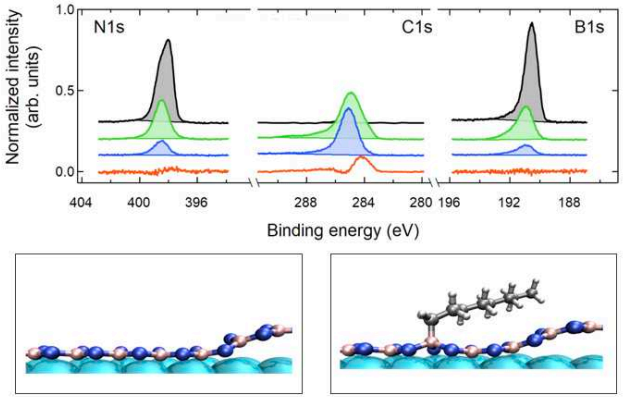
Prof. Thomas Greber

We study objects like **zero dimensional endofullerene** molecules and **two dimensional (2D) boron nitride** layers in view of their functionality as nano-materials.
Single molecule magnetism is the focus in the fullerene research, where we apply bulk sensitive x-ray absorption and a sub-Kelvin superconducting quantum interference device for the investigation of the materials that are obtained from collaborations with synthesis groups.
In the 2D materials activity we aim to grow highest quality boron nitride on substrates with chemical vapour deposition methods and subsequent exfoliation. For this purposes we use a clean room, optical microscopy, transmission electron microscopy and surface science methods such as low energy electron diffraction, photoemission and scanning tunneling microscopy for our investigations.

https://www.physik.uzh.ch/g/osterwalder

Catalyst Proximity-Induced Functionalization of $h-$BN

A single layer boron nitride realises a membrane that separates two regions. Still, such membranes allow chemical interaction across the layer. As we showed this year [1] one layer of $h-$BN on rhodium does not suppress the catalytic action of the rhodium substrate, which is reminiscent to proximity effects as they are observed in magnetic interfaces or in superconductors. We investigated with high resolution x-ray photoelectron spectroscopy (XPS) the interaction tetraoctylammonium (TOA) ions with $h-$BN/Rh(111). While the electrochemical process enables the large scale exfoliation of single layer $h-$BN, the underlying mechanism was not understood. XPS before and after TOA treatment in the liquid phase and density functional theory detailed a picture where the proximity of the substrate on which $h-$BN was grown is essential for the processes at work. The results as summarised in the Figure indicate that TOA may dissociate and that part of the resulting octyl radicals bind on the top face of $h-$BN but do not intercalate between the interface of $h-$BN and



Experimental XPS spectra of nitrogen, carbon and boron on h-BN/Rh(111) before (black) and after TOA treatment at normal emission (green), and at 84° grazing emission (blue). The differences between green and blue are depicted in orange. The photon energy is 850 eV, and all signals are normalised with their corresponding photoemission cross sections. The grazing angle data are scaled with a factor of 5.7 such that the carbon peak heights coincide. Bottom panels: Cross-sectional views of structures from XPS calculations before and after TOA treatment. The octyl radicals bind to a boron atom (pink) in the h−BN nanomesh pores.

rhodium. This functionalization scheme realises $h-$BN Janus membranes with two distinct faces which may become of use for biasing the transport direction of ions across such membranes.

Due to the required kinetic energy and resolution of the photoelectrons the XPS experiments were performed at the photoemission and atomic resolution laboratory (PEARL) beamline at the Swiss Light Source of the Paul Scherrer Institut.

This activity is supported by the European Future and Emerging Technology Flagship graphene.

Highlighted Publications:

1. Catalyst Proximity-Induced Functionalization of $h-$BN with Quat Derivatives
   A. Hemmi *et al.*, Nano Letters **19**, 5998 (2019)
2. Circular dichroism and angular deviation in x-ray absorption spectra of $Dy_2ScN@C_{80}$ single-molecule magnets on *h*-BN/Rh(111)
   T. Greber *et al.*, Phys. Rev. Mat., **3**, 014409 (2019)
3. Production and processing of graphene and related materials
   C. Backes *et al.*, 2D Mater., **7**, 022001 (2020)

Quantum Matter

Prof. Fabian Natterer

Our research investigates how matter receives her properties from the interaction between individual atoms. We especially focus on artificially built quantum matter that we assemble from scratch, one atom at a time. Our scanning tunneling microscope hereby serves as a tool for the construction of atomic structures and the characterization of its emergent properties. We use this knowledge to steer interesting quantum behavior, such as magnetic monopole excitations. We furthermore study 2D van der Waal materials and develop new measurement protocols for advanced scanning probe microscopy investigations, such as electron spin resonance and compressed sensing for quasiparticle interference mapping.

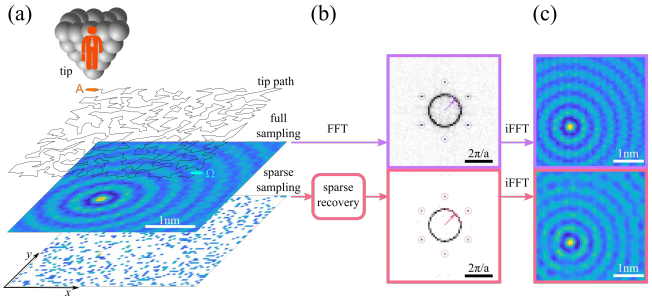
https://www.physik.uzh.ch/g/natterer

Scanning Probe Microscopy based ESR

One of our main projects is the development of Scanning Probe Microscopy based Electron Spin Resonance (ESR) and pump-probe methods to investigate the dynamics of single atom magnets. Using pulsed ESR, we gain control over the quantum phase of an atomic qubit that serves as a powerful quantum sensor for magnetic signatures at the atomic scale, such as in our artificially built quantum matter. Pump-probe methods yield insight into the lifetime of magnetic states, which defines the limits for data conservation and quantum manipulation.

Compressed sensing methods

The introduction of compressed sensing (CS) methods for scanning probe measurements is our second major project. Compressed sensing can fundamentally speed up measurements (ten to hundred-fold), because it removes data redundancies and requires only the mea-



Measure smarter, not harder, it the guiding principle behind our compressive sensing methods. The sparsely sampled LDOS allows perfect reconstruction of the QPI information with only a fraction of the usual measurements.

surement of a fraction of the full dataset. The applicability of CS is given for any data that is sparse in some represation domain. This is the case in many quasiparticle interference (QPI) measurements, where the number of wavevectors is typically significantly smaller than the number of data points. Traditional QPI may take up to hundreds of hours, whereas CS can retrieve the same information in a fraction of this time. The shorter measurement time allows us to better use our resources to improve the spectroscopic resolution which may help identify finer band-structure details of exotic 2D materials.

Highlighted Publications:

1. Sparse Sampling for Fast Quasiparticle Interference Mapping
   J. Oppliger and F.D. Natterer, arXiv 1908.01903 (2019)
2. Waveform-sequencing for scanning tunneling microscopy based pump-probe spectroscopy and pulsed-ESR,
   F.D. Natterer, arXiv 1902.05609 (2019)
3. Quantum state manipulation of single atom magnets using the hyperfine interaction
   P. Forrester *et al.*,arXiv 1903.00242 (2019)

Surface physics

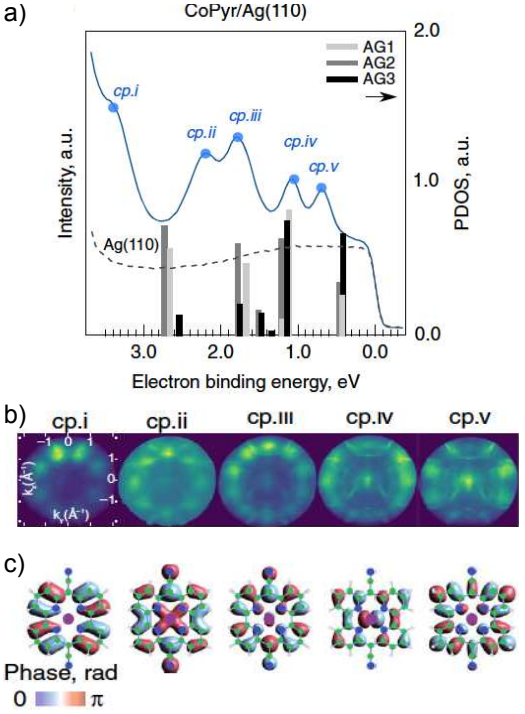
Prof. Jürg Osterwalder

We study processes at surfaces such as molecule adsorption and self assembly, charge and energy transport as well as fundamental aspects of **light-matter interaction** and associated electronic and atomic dynamics. Our laboratory is equipped with a toolbox of surface science methods for the preparation and characterization of clean single-crystalline surfaces that can be used to investigate such phenomena **at the atomic and molecular level**. Specific research projects include the structure and function of adsorbed catalyst molecules on semiconductor surfaces that serve as model electrodes in water splitting devices, as well as the measurement of molecular orbitals of adsorbed donor-acceptor dyads and their charge-transfer dynamics by **orbital tomography**. Finally, we push the development of new experimental techniques, most recently ambient-pressure XPS at **solid-liquid interfaces** at the Swiss Light Source at PSI.

https://www.physik.uzh.ch/g/osterwalder

Identifying molecular orbitals of adsorbed molecules by angle-resolved photoelectron spectroscopy

Valence electrons in molecules form delocalized molecular orbitals (MOs) which determine their physical properties and chemical reactivity. The energies of the MOs are sensitive to the local environment of the molecule such that, for instance, the ordering of the binding energies can change when molecules are adsorbed on a metal surface. UV excited photoelectron spectroscopy (UPS) can measure the energy distribution of MOs, but for the assignment of a measured energy level to a particular molecular orbital, one needs to go one step further. The angular distribution of the photoelectron intensity of a particular peak in the UPS spectrum carries the signature of the associated MO. Under certain conditions, it has been demonstrated that the MO can be directly reconstructed from the angular distribution map via a Fourier transform method including iterative phase retreaval algorithms, an approach termed *orbital tomography*.



a) UV photoelectron spectrum of a monolayer of Co-pyrphyrin molecules on an Ag(110) surface. b) Photoelectron angular distribution maps from molecular orbitals as denoted in a). c) Phased isosurfaces of corresponding molecular orbital amplitudes.

One condition necessary for this approach to work is that all molecules within the macroscopic probing area on the sample are adsorbed in a single orientation. However, adsorbed molecules often arrange themselves in domains with different orientations. In a collaboration with the Department of Chemistry of UZH we studied the system of Co-pyrphyrin on the Ag(110) surface. MOs were calculated via density functional theory and Fourier transformed in order to obtain their angular distribution maps. Superpositions of these maps with different orientations could be fitted to the measured maps for an unambiguous identification of five different MOs.

Highlighted Publications:

1. Comparative study of different anchoring of organometallic dyes on ultrathin alumina, W.-D. Zabka *et al.*, J. Phys. Chem. C **123**, 36 (2019)
2. Polarization-sensitive reconstruction of transient local THz fields at dielectric interfaces, K. Waltar *et al.*, Optica **6**, 1431 (2019)
3. Combined orbital tomography study of multi-configurational molecular adsorbate systems, P. Kliuiev *et al.*, Nature Commun. **10**, 5255 (2019)
4. Sb_2Se_3(100): A strongly anisotropic surface, R. Totani *et al.*, Phys. Rev. Materials **3**, 125404 (2019)

Phase Transitions, Materials and Applications

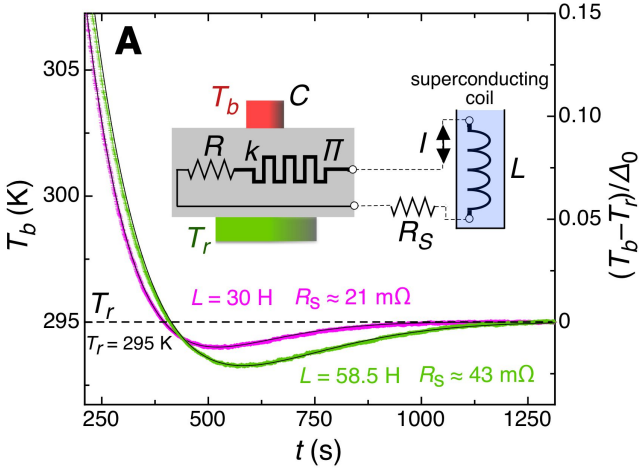
Prof. Andreas Schilling

We are interested in selected topics in materials research, spanning the entire spectrum from **searching new materials**, their **characterization**, and corresponding **applications**. We have been particularly active in **superconductivity, magnetism and thermodynamics**. Our laboratory is equipped with modern furnaces for material synthesis, various ^{4}He/^{3}He cryostats and a dilution cryostat, all with superconducting magnets. We are structuring thin superconducting films at the FIRST Center for Micro- and Nanoscience at ETHZ and are using them both for basic research and applications. While the physics of thin-film superconductors is a fascinating research topic by itself, corresponding nanostructures may serve as ultrafast single-photon detectors in the infrared, visible and X-ray range.

https://www.physik.uzh.ch/g/schilling

Design and implementation of a "thermal inductor"

Heat currents and electrical currents can both be described with the same mathematical formalism. The electric analogue to a heat current is the electric current; heat corresponds to charge, and temperature to voltage; an electric capacitor is equivalent to a heat capacity, and electric conductivity corresponds to thermal conductivity. However, no thermal analogue to an inductor has been reported up to present. It has been argued that its existence would violate the second law of thermodynamics, because a corresponding thermal LC circuit could carry an oscillating heat current where the temperature difference between two bodies perpetually changes its sign, and heat would temporarily flow form the colder to the warmer object. We have shown already in 2011 that a Peltier element, switched in series with an electric inductor and connected with a heat capacity, behaves like a thermal LC circuit with certain a "thermal inductance". When operated entirely passively, only over-damped temperature oscillations were expected at that time. A detailed analysis of the circuit



Temperature undershoot during the first cycle of a damped temperature oscillation, starting from 100° C at t = 0.

showed, however, that a careful choice of superconducting inductors (L) and efficient Peltier elements (Π) allows for true temperature oscillations. In a typical experiment, an object (C) is initially heated and then connected to one side of the Peltier element, with a heat bath held at ambient temperature (T_r) on its other side. After a while, the temperature T_b of the object indeed dropped below that of the thermal bath. The maximum temperature difference to ambient temperature reached only 2 °C, however, which was mainly limited by the performance of the commercial Peltier element. Under the same conditions, a cooling from 100 °C down to -47 °C could be theoretically achieved, which would require the use of an ideal Peltier element with maximum possible efficiency. In theory, large amounts of a hot material could be cooled well below room temperature in this way, without any energy consumption or moving parts, and the passive thermal circuit could be used as often as desired. Most remarkably, heat is directed directly from the cold to the warm object for some time in such experiments, without being temporarily stored as magnetic energy in the electric inductor, and the process, which passes through a series of quasi-equilibrium states, still obeys the second law of thermodynamics. To prove this, we showed that entropy of the whole system is strictly monotonically increasing with time. Finally, we identified a very general thermodynamic limit for the maximum possible cooling effect that can occur during any thermal oscillation cycle without external work done on a system.

Highlighted Publications:

1. Heat flowing from cold to hot without external intervention by using a “thermal inductor”,
A. Schilling, X. Zhang, and O. Bossen,
Science Advances 5, eaat9953 (2019)
Popular summary:
https://www.youtube.com/watch?v=4Vi8k-p4COY