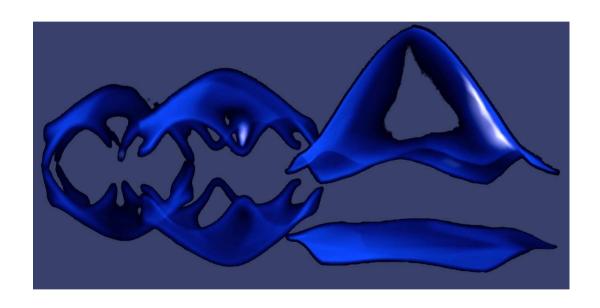
Condensed Matter Physics



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.

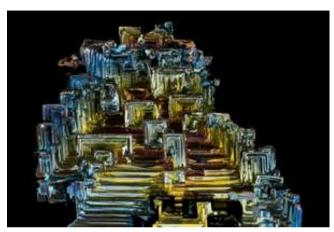
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Higher-order topology: Electrons living on the edge

Topology is a field of mathematics that fascinates physicists more and more in recent years. It is concerned with properties that are particularly robust against perturbations and deformations. For about ten years we know a class of materials called topological insulators, which are crystals that are insulators in the bulk but conduct electrical current on their surface. The conducting surfaces are topologically protected, which means that they cannot be brought into an insulating state easily.

Recently, we studied a new class of topological insulators which do not possess conducting states on the surface, but on the hinges of a crystal. We dubbed the new material class "higher-order topological insulators". The extraordinary robustness of the conducting hinges makes them particularly interesting: for instance, they cannot be removed by adding disorder or impurities. If a crystal imperfection gets in the way of the current of topological electrons, this



Bismuth is not only visually appealing but has also interesting electronic properties, as the group of Titus Neupert has uncovered in their recent work.

current is not stopped but simply flows around the impurity.

The crystal hinges do not have to be prepared in a special way in order to conduct current. If one breaks the crystal, one obtains new hinges that are automatically conducting in this topological way. Most exciting is the fact that theoretically the electric conduction happens without dissipation, i.e., without resistance. This property, which is otherwise known from superconductors at low temperatures, cannot be found in topological insulators with conducting surface states. One

can think of the crystal hinges as forming a highway for electrons, on which they cannot make a U-turn.

One hope is that nanowires made of higher-order topological insulators may serve as current paths in electric circuits in the future. Furthermore, they may be combined with magnetic and superconducting elements to serve as quantum bits in future quantum computers. To make progress toward these visions, the new class of materials has to be thoroughly studied theoretically and experimentally. We theoretically proposed tin-telluride as a compound that should show these novel phenomena. Furthermore, in a collaboration with two experimental groups from Princeton and Paris, we were able to show that elementary bismuth is a higher-order topological insulator.

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 - S. Imhof et al., Nature Physics 14, 925–929 (2018)
- 3. Higher-order topological insulators, F. Schindler *et al.*, http://advances.sciencemag.org/ content/4/6/eaat0346.full.pdf

Computational materials theory

Prof. Alexey Soluyanov



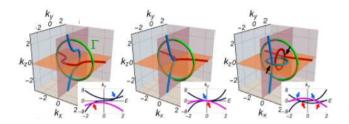
Our research is aimed to prediction of materials that host topological phases. This is done by computing special kind of quantum numbers called topological invariants. These invariants contain information about the geometric properties of the wave functions that describe the state of material. In metals they describe topologically protected band degeneracies in the vicinity of the Fermi level that govern the excitations of topological metals and lead to transport properties not seen in ordinary metals. In topological insulators these invariants describe the metallic surface or edge states of materials with insulating bulk. Topological materials hold big promise for quantum technologies.

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Novel topological phases in simple metals

We established a novel approach to uncover constraints put on the behavior of electronic bands in metals that have a PT-symmetry, that is the product of inversion and time reversal. These constraints are described by topological invariants, which unlike all the known to date cases form a non-Abelian group. The invariants describe nodal lines (paths in momentum space, along which two electronic energy bands are degenerate) and their non-Abelian nature uncovers the impossibility of interchanging two nodal lines described by different invariants from the group without forming other nodal lines, not present in the material before. We also made a material prediction for experimental verification of this theory. Elemental metal – scandium – hosts nodal lines below the Fermi level that under certain epitaxial strains interchange in exact accord with our theoretical prediction. As illustrated in the figure, blue and red nodal lines, formed by different bands, are pushed across each other by strain, but once interchanged both of them obtain additional nodal lines that form



Interchange of two nodal lines in momentum space: The red and blue nodal lines with different topological charges are separated from each other before the exchange (left), then under strain meet each other (central), and move across each other (right), forming two additional nodal lines enforced by non-Abelian topology that is tracked by a special invariant, computed on the green loop Γ .

ear-like loops, because the red and blue nodal lines have topological charges described by the non-commuting topological invariants from the non-Abelian group. The discovery of non-Abelian topological charges (invariants) allowed us to introduce a topological phase that goes beyond the classification schemes that were standard in the field of topological materials.

While non-Abelian topology is usually associated with a special kind of two-dimensional quasiparticles called non-Abelian anyons that unlike fermions and bosons obey fractional exchange statistics in coordinate space, this work provides the first illustration of non-Abelian topology in momen-

tum space. Realization of non-Abelian anyons is only possible in the presence of strong interactions or superconductivity, and these quasiparticles are predicted to be the cornerstone of topological quantum computing. Non-Abelian nodal lines described in our work can be realized in the most simple crystalline metals, but still holds technological promises, due to the possibility to create topologically protected doublets on the ends of insulating quantum wires, which follows from our derivations. The detailed study of such wires and their properties is left for future work.

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 - Q. S. Wu, A. A. Soluyanov,
 - T. Bzdusek, arXiv:1808:07469
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- Automated construction of symmetrized Wannier-like tight-binding models from ab initio calculations,
 D. Gresch, Q. S. Wu, R. Hauselmann, M. Troyer,
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Surface physics

Prof. Jürg Osterwalder

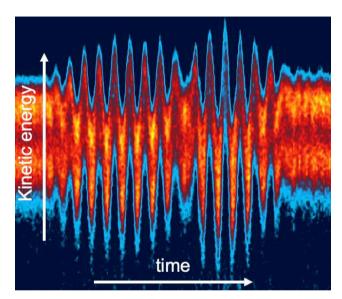


We study processes at surfaces such as molecule adsorption and self assembly, charge and energy transport as well as fundamental aspects of light-matter interaction and associated electronic and atomic dynamics. Our laboratory is equipped with a toolbox of surface science methods for the preparation 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 chargetransfer dynamics by orbital tomography. Finally, we push the development of new experimental techniques, most recently ambient-pressure x-ray Photoelectron Spectroscopy (XPS) at solid-liquid interfaces at the Swiss Light Source at PSI.

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Measuring local fields of ultrashort terahertz pulses at surfaces

The oscillating electric fields of intense terahertz (THz) pulses can be used to excite specific low-frequency modes in condensed matter or drive confined alternating currents in nanostructured arrays, paving the way for a new class of optoelectronic devices. The strong interaction leads to strong modifications of the THz fields in the vicinity of surfaces and interfaces. Our group has developed a method that measures these local fields by exciting photoelectrons at the surface with extreme ultraviolet radiation (XUV) pulses and by observing the effect that the THz field has on their kinetic energy and momentum. Varying the temporal delay between the XUV and THz pulses leads to photoelectron streaking traces as shown in the figure. Here, the kinetic energy of the electrons is periodically modulated by the acceleration/deceleration in the oscillating THz field component perpendicular to the surface. The energy oscillations are thus a direct consequence of the interaction of the electron with the THz standing-wave field that builds up close to



Electrons dance in the rhythm of the electrical field within a terahertz pulse after being photoemitted by an extreme ultraviolet pulse. The color code represents the measured photoemission intensity of platinum valence levels (yellow = high).

the surface during the THz pulse duration of a few picoseconds. In our method, we further exploit the two-dimensional detection system of our spectrometer that measures the kinetic energy and the polar emission angle of the photoelectrons concurrently. From the latter we can extract also the THz field component parallel to the surface.

Our motivation for this study was to explore the idea that strong THz fields might induce chemical reactions at surfaces and thus enhance the activity of a catalyst. As a case study we selected carbon monoxide molecules on a platinum surface. One can expect the THz field to couple to the electrical dipole moment of adsorbed CO molecules, thus inducing molecular motion and chemical dynamics. For these experiments, we had to bring our angle-resolved photoelectron spectrometer to the FLASH free-electron laser at DESY in Hamburg, where XUV light and THz radiation is available at the same beamline, produced by two consecutive undulators. Our measurements showed that the THz fields at the surface were too weak to induce any structural dynamics.

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- 2. Algorithms and image formation in orbital tomography, P. Kliuiev *et al.*, Phys. Rev. B **98**, 085426 (2018)
- Polarization-sensitive pulse reconstruction by momentum-resolved photoelectron streaking, K. Waltar *et al.*, Opt. Express 26, 8364-8374 (2018)

Low dimensional systems

Prof. Thomas Greber



We study objects like **zero dimensional endofullerenes** and **two dimensional (2D) boron nitride** 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 to the materials that we obtain from collaborations with synthesis groups.

In the 2D activity we aim to **grow highest quality boron nitride** on substrates with chemical vapour deposition methods and subsequent **exfoliation** of single layers. 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.

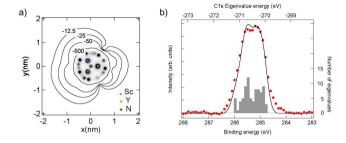
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Electrostatic Interaction across a Single-Layer Carbon

Low dimensional systems like single layer boron nitride or fullerenes, both realise membranes that separate two regions. Though these ultimately thin single layer membranes allow chemical interaction across the membrane. For example, electrons may easily tunnel across single layer boron nitride, or the carbon cage of a fullerene molecule does not realize a Faraday cage that completely shields the electrostatic field of the endohedral unit [1]. This is reminiscent to proximity effects as observed in magnetic interfaces or in superconductors. It is a manifestation of physics at the nanometer scale and may possibly be exploited in future nanodevices. In the case of magnetic endofullerenes electrostatic control will open new possibilities of addressing the spin information inside the molecules.

Specifically, we investigated the single molecule magnet $TbSc_2N@C_{80}$ [1]. Over all, the molecule is neutral and has a very small dipole moment. The $TbSc_2N$ endohedral unit transfers six electrons on the carbon cage. The resulting



Electrostatic potential of a C_{80} endohedral fullerene. (a) Calculation of the potential of $YSc_2N@C_{80}$ on a plane comprising the endohedral cluster and the carbon shell (contour units meV). (b) High resolution x-ray photoelectron spectroscopy from the carbon shell of $TbSc_2N@C_{80}$ (red dots) and comparison to the calculated C1s eigenvalues that mainly reflect the electrostatic potential at the 80 carbon sites (grey bars and black line) (from [1]).

discrete charge distribution causes an electrostatic potential that is not spherical and thus not constant outside the molecule. The figure above shows the calculated electrostatic potential. As expected, it falls off rapidly but has a significant non-isotropic component outside the carbon cage. The potential in the immediate vicinity of the cage may not be measured easily, though it can be inferred from the potential at

the positions of the carbon atoms. The potential variation on the carbon cage is reflected in the electron binding energies as they are measured with photoemission. We could establish the correlation between the calculated C1s eigenvalues and the measured C1s core level binding energies. Due to the high requirements to the energy resolution the experiments were performed at the photoemission and atomic resolution laboratory (PEARL) beamline at the Swiss Light Source.

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 - R. Stania et al., J. Phys. Chem. Lett. 9 3586 (2018)
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 - B. Salzmann *et al.*, J. Vac. Sci. Technol. A **36** 020603 (2018)
- 3. Centimeter-sized single-orientation monolayer hexagonal boron nitride with or without nanovoids H. Cun *et al.*, Nano Letters **18** 1205 (2018)
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Phase Transitions, Materials and Applications

Prof. Andreas Schilling



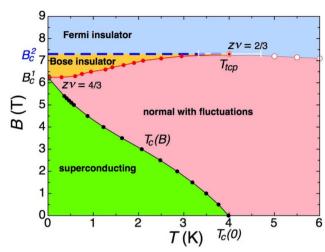
We are interested in selected topics in materials research, spanning the entire spectrum from searching new materials, their characterization, and corresponding applications. We have been particularly active in superconductivity, magnetism and thermodynamics. Our laboratory is equipped with modern furnaces for material synthesis, various 4He 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 thinfilm 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.

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The advantages of amorphous WSi

We have been working with ultrafast superconducting nanowire single-photon detectors since more than a decade, with the aim to detect single photons in the visible, in the infrared, and even in the X-ray range. In the early stages, efforts concentrated on the deposition of high-quality crystalline or granular superconducting thin films. We realized later on that very homogeneous superconducting films can be easily obtained with amorphous superconductors. Due to their uniformly amorphous nature on a microscopic scale, an electrical current is naturally homogeneously distributed in such films, which makes them perfectly suitable for the research on superconductivity in nanostructures. They are also very suitable for device fabrication because constriction effects can be essentially neglected. Indeed, the highest detection efficiency so far was obtained in 4-nm-thick amorphous WSi films. These amorphous superconductors are very robust against chemical degradation, and can also be deposited on a variety of substrates, even on glass or photon resists.



Sketch of the superconductor-to-insulator transition the magnetic phase diagram of an amorphous 5nm thin WSi film.

Magnetic phase diagram of amorphous WSi thin films

In general, a zero-temperature magnetic-field-driven superconductor to insulator transition (SIT) is expected to occur in quasi-two-dimensional superconductors when the applied magnetic field crosses a certain critical field. A fundamental question is whether this transition is due to the localization of Cooper pairs or due to their destruction of. We have addressed this question by studying the SIT in an amorphous WSi film with a thickness of ≈ 5 nm. Transport measurements revealed the localization of Cooper pairs at a quantum critical field B_c^1 (Bose insulator), with a product of the correlation length and dynamical exponents $z\nu \sim 4/3$ near the quantum critical point. Beyond B_c^1 , superconducting fluctuations still persist at finite temperatures. Above a second critical field $B_c^2 > B_c^1$, the Cooper pairs are destroyed and the film becomes a Fermi insulator. The different phases all merge at a tricritical point at finite temperatures with $z\nu = 2/3$. These results suggest a sequential superconductor to Bose insulator to Fermi insulator phase transition, which differs from the conventional scenario involving a single quantum critical point.

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- 2. Sequential superconductor-Bose insulator-Fermi insulator phase transitions in quasi-2D α -WSi,
 - X. Zhang and A. Schilling, Phys. Rev. B **97** 214524 (2018)
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 - X. Zhang et al., Phys. Rev. B 97 174502 (2018)

Superconductivity and Magnetism

Prof. Johan Chang

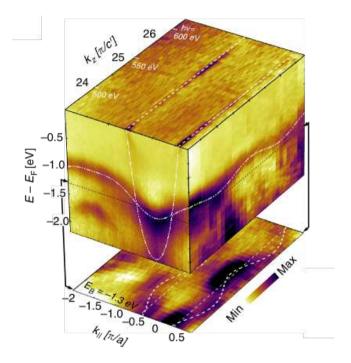


We investigate quantum matter phases emerging from strong electronic interactions. High-temperature superconductivity, strange metals, density-wave instabilities and electronic driven metal-insulator transitions are studied by synchrotron and laboratory based experimental techniques. At international 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.

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Distilling Electrons for Superconductivity

The minimal ingredients to explain the essential physics of layered copper-oxide (cuprates) materials remain heavily debated. Identifying the factors that limit the transition temperature T_c of high-temperature cuprate superconductivity is a crucial step towards revealing the design principles underlying the pairing mechanism. It may also provide an explanation for the dramatic variation of T_c across the known singlelayer compounds. Although superconductivity is certainly promoted within the copper-oxide layers, the out-of-plane apical oxygen position may play an important role in defining T_c . It has, for example, been predicted that apical oxygen distance influences T_c in at least two different ways. First, the apical oxygen distance d_A to the copper-oxide plane controls the charge transfer gap between the oxygen and copper sites which, in turn, suppresses superconductivity. Second, Fermilevel orbital hybridisation, controlled by d_A , impedes superconductivity. For the latter scenario, no double orbital electronic structure has been observed. In the quest to disentangle



Three-dimensional band structure of the high-temperature superconductor $La_{2-x}Sr_xCuO_4$ measured by angle-resolved photoemission spectroscopy.

these causal relation between d_A and T_c , it is therefore imperative to experimentally reveal the orbital character of the cuprate band structure. We have performed direct ultraviolet and soft-x-ray ARPES measurements of the electronic structure of La-based single-layer compounds. A double orbital electronic band structure with direct hybridisation has been identified.

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 Das et al., Physical Review X 8 11048 (2018)
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Oxide Interface Physics

Prof. Marta Gibert



Epitaxial heterostructures allow for multiple strategies to manipulate the interplay between the different degrees of freedom in transition metal oxides. Reduced dimensionalities and interfacial structural and electronic couplings are key to tune the properties of these materials and even allow the engineering of novel functionalities.

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

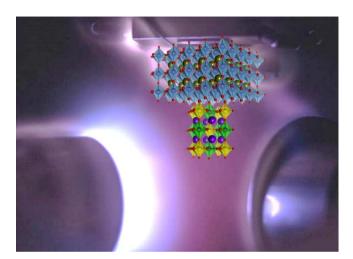
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Transition metal oxides (TMOs) are an extensive class of compounds showing an incredible variety of physical properties such as metal-insulator transitions, exotic magnetism, multiferroicity, superconductivity and many more.

This places them as interesting candidates for next generation electronic devices. All these unique properties stem from strong electronic correlations and a complex interplay between the charge, orbital, spin and lattice degrees of freedom.

These materials often crystallise in rather similar structures made of simple building blocks consisting of a transition metal (B) embedded in an oxygen octahedral cage in the perovskite ABO₃ structure. As a result, and thanks to the advances in growth techniques, it is today possible to stack layers of different TMO compounds one on top of the other (just like *lego*-blocks) with atomic scale precision. These new artificially layered structures are very interesting because they allow not only the bulk functionalities to be further tuned, but also because they often pave the way to novel electronic properties completely different to those of the parent compounds. Landmark examples include the emergence of conductivity at the interface between insulators or ferromagnetism between antiferromagnets. This flourishing research field is called **oxide interface engineering**.



Plasma during the growth (upside down) of a La_2NiMnO_6 thin film by off-axis rf sputtering. The double-perovskite-film/perovskitesubstrate heterostructure is sketched.

In our group, we study the structure-property relation in TMOs when grown into atomically-engineered layered heterostructures (i.e. thin films or superlattices). To that aim, we have built up an off-axis rf-magnetron sputtering deposition system which allows high quality oxide heterostructures to be generated. During this first year at UZH, in addition to study the perovskite nickelates, we have started developing

a new research line focused on double-perovskite $A_2BB'O_6$ structure films, where the ordered rock-salt like arrangement of corner-sharing BO_6 and $B'O_6$ units allow for an additional knob to control the functionalities of TMOs.

Special attention has been given to La₂NiMnO₆, an insulator ferromagnet with almost room temperature transition temperature ($T_c \sim 280 \, \text{K}$) in bulk. Ferromagnetic insulators are rare in nature, given that ferromagnetism is often accompanied by metallicity. However, ferromagnetic insulators are needed for a variety of devices in fields such as spintronics. We have showed that long-range order of Mn⁺⁴-Ni⁺² cations and the magnetic properties of bulk can be achieved in films of only few nanometres thickness. Careful optimization of the growth conditions and detailed characterization through a variety of techniques (x-ray diffraction, atomic force microscopy, SQUID-magnetometry, absorption spectroscopy, etc.) is key to our research.

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 - S. Catalano, M. Gibert, et al.
 - J. Reports on Progress in Physics 81 046501 (2018)

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 quantum point interference mapping.

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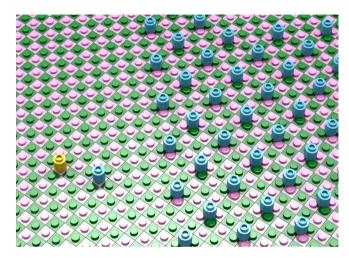
Scanning Pulse Microscope

One of our main projects is the development of pulsed electron spin resonance (ESR) and pump-probe methods for the

scanning tunneling microscope 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 other project. Compressed sensing can significantly speed up measurement times (ten to hundred-fold), since only a subset of data needs to be recorded provided the information content is sparse. This is the case in many quantum point interference (QPI) measurements, where the number of wavevectors is typically significantly smaller than the number of data points. Traditional QPI may take up to



Understanding the interaction between two atoms is the first step towards building artificial quantum matter.

hundreds of hours, whereas CS can retrieve the same information in a fraction of this time. The shorter measurement time allows us to reinvest time to improve our spectroscopic resolution which may help identify more band-structure details of exotic 2D materials.

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- 4. Waveform-sequencing for scanning tunneling microscopy based pump-probe spectroscopy and pulsed-ESR,
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- 5. A quantum pathway to overcome the trilemma of magnetic data storage,P. Forrester *et al.*, arXiv 1903.00242 (2019)

Disordered and biological soft matter

Prof. Christof Aegerter



We study the properties of disordered and heterogeneous systems out of equilibrium. This encompasses **light transport in turbid substances**, the dynamics of levitated foams as well as the elastic properties of growing biological tissues, such as *Drosophila* embryos and wing discs and their influence on development.

In all these fields our investigations are mainly experimental, however we also use computational modeling to guide these experiments.

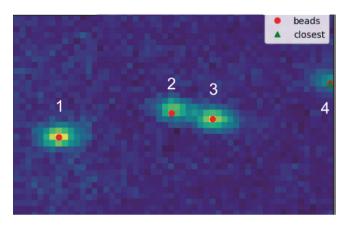
Our studies of light transport in disordered media have two main foci consisting of enabling imaging in turbid media, where we use wave-front shaping of the light to counter-act the effects of multiple scattering and the production of colouration due to scattering rather than pigmentation in photonic glasses and natural systems.

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Imaging behind turbid media: Extending the field of view

Turbid media, such as fog, milk or white paint are detrimental to imaging because light passing through them is multiply scattered and hence directional information is lost. Due to the wave nature of light, it is however possible to obtain information about the scattering process encoded in the spatial interference (speckle) pattern formed behind the turbid medium. Using this knowledge and adjusting the incoming wave-front accordingly using a spatial light modulator, it is possible to create a focused laser beam even behind thick layers of white paint. In this, the disorder inherent in the multiple scattering is actually used to create the focus via constructive interference akin to the use of destructive interference in noise cancelling headphones.



Imaging of fluorescent particles behind a layer of white paint, where the field of view is extended in excess of the theoretically possible range dictated by the optical memory effect.

A scanning of this focus is possible due to the optical memory effect, which prescribes that a shift over an angular range given by the ratio of the wavelength to the thickness can be achieved. Using this method, we have previously shown that diffraction limited imaging of fluorescent particles is possible even behind layers of white paint much thicker than the mean free path. The applicability of this is however limited.

ited due to the limited field of view of the imaging implied by the range of the memory effect. Using an iterative approach, we have now shown that this limitation can be overcome, which is shown in the Figure on the left side, where an image of fluorescent particles is shown over a field of view exceeding the memory effect range by a factor of three. Hence microscopy behind turbid media comes into the realm of being technically feasible.

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- 3. Enhanced field of view scattered light fluorescence microscopy,
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