CUI WINTER SCHOOL 2016

Todtmoos (Germany), February 15-19, 2016

3rd Winter School of
The Hamburg Centre for Ultrafast Imaging

DESY European XFEL MAX-PLANCK-GESELLSCHAFT Universität Hamburg DER FORSCHUNG | DER LEHRE | DER BILDUNG EMBL DFG

The Hamburg Centre for Ultrafast Imaging

How do the elementary building blocks of nature move? Can atoms, molecules and electrons in matter be controlled and driven with precision on all length and time scales?

These questions represent some of the biggest and most exciting challenges of modern science – and the central objective of The Hamburg Centre for Ultrafast Imaging (CUI): The analysis of fundamental chemical and physical processes in Photon and Nano Science.

The scientists of CUI hope to gain profound insight into fundamental phenomena such as the mechanisms of high temperature superconductivity, the appearance of different states of magnetism or the development of ordered molecular as well as biological and mesoscopic structures. The expected insights will extend and broaden our understanding of physics, chemistry and biology and will result in new applications in medicine and novel materials for key technology areas.

Research Area A - Imaging and Control of Quantum Systems

For a full understanding of structural dynamics, one needs information on the electronic as well as the nuclear degrees of freedom. This research focus uses advanced optical imaging techniques to identify key enabling features for controlling quantum state evolution. We envisage the possibility to control chemistry along the ground state electronic surface to open up all classes of

molecular systems to atomic level inspection. The system size is scaled up from small molecules to collective effects in solid state or periodic media and includes the systematic study of isolated molecules with small potential barriers separating different structures but also takes into account a variable coupling of a system to the environment. With a detailed understanding of electronic coupling to the bath we shall be able to control coherence and degree of dissipation to the point of controlling material properties. For the case of highly correlated electron-lattice systems, this knowledge will lead to new means to control coherence and macroscopic properties with the prospect to eventually create transient superconducting states at high temperatures. The design of novel materials with unique properties is greatly aided by our capabilities to build fully controllable quantum simulators based on periodic structures formed in ultracold quantum gases. In these analog quantum processors ultracold matter is tailored to mimic magnetism and superconductivity under idealized conditions. Apart from the long range correlation effects governing material properties, there is a deep fundamental issue related to the role of quantum information transport in such highly quantized systems. To this end, we are studying the coherence properties of matter waves escaping from a macroscopic quantum object like a Bose-Einstein condensate.

Research Area B - Atomically Resolved Structural Dynamics

A particular dream experiment is to directly watch atomic motions during a chemical event, such as a bond breaking. With the advent of ultrabright electron and x-ray sources, this has become possible.

Techniques such as coherent imaging will allow us to directly watch atomic motions in complex systems, such as in a biological reaction or collective dynamics in a condensed matter system. In this research area we bring together multidisciplinary expertise in laser science, structural biology, chemistry, molecular physics, and imaging science and focus on the basic underlying concepts of systems from small molecules to amino acids and to protein complexes.

Research Area C – Dynamics of Order Formation on the Nanoscale

Research Area C extends the length scale of interest from the molecular level to the nanoscale where collective effects play a defining role in material properties. The study of ultrafast ordering phenomena and nucleation events is not only crucial for understanding these materials but also for the development of tools for nanoscience. With the new X-ray light sources ordering and nucleation can be investigated down to fundamental time scales of atom mobility in solids and solution, covering even short-living transient states. Research Area C is divided into three different Research Foci which focus all on time resolved investigations of ordering phenomena on the nanoscale. RFC.1 addresses the role of transient structures in molecular liquids such as water as well as the role of structural and orientational correlations for the glass transition. In RFC.2 we study nucleation and growth processes of nanoparticles and correlate their shape and phase transformations with external triggers. The subject of RFC.3 is the study of ultrafast spin ordering processes in nanostructures under the influence of dipolar and exchange interactions.

Timetable & Program

Monday

16:00 Arrival and Welcome

17:30 PhD Talks: Session 1

19:30 Free Time

20:00 Dinner

Tuesday

07:30 Breakfast

08:30 PhD Talks: Session 2

10:30 Coffee Break

11:00 Courses C: General + Advanced

Prof. Dr. Simone Mascotto (Hamburg) – Nanoporous Solids

Dr. Jörg Polte (Berlin) – Fundamental Principles of Nanoparticle Formation

13:00 Lunch

16:30 Coffee

17:00 Courses A: General + Advanced

Prof. Dr. Jochen Küpper (Hamburg) – Light-Matter Interaction

Prof. Dr. Matthias Wollenhaupt (Oldenburg) – Coherent Control of Ultrafast Processes in Molecular Dynamics

19:00 PhD Talks: Session 3

20:00 Dinner

Wednesday

07:30 Breakfast

08:30 Courses A: General + Advanced

Prof. Dr. Jochen Küpper (Hamburg) – Light-Matter Interaction

Prof. Dr. Matthias Wollenhaupt (Oldenburg) – Coherent Control of Ultrafast Processes in Molecular Dynamics

10:30 Coffee

11:00 Courses C: General + Advanced

Prof. Dr. Simone Mascotto (Hamburg) – Nanoporous Solids

Dr. Jörg Polte (Berlin) - Fundamental Principles of Nanoparticle Formation

13:00 Lunch

16:00 Coffee

16:30 Courses B: General + Advanced

Prof. Dr. Henning Tidow (Hamburg) – Proteins: Structure and Function

Dr. Robin Owen (Didcot, UK) – X-ray Crystallography: From Electrons in an Undulator to Electrons in a Crystal

18:30 PhD Workshops: Connect and discuss research projects with others. Speakers welcome.

20:00 Dinner

Thursday

07:30 Breakfast

08:30 Courses B: General + Advanced

Prof. Dr. Henning Tidow (Hamburg) – Proteins: Structure and Function

Dr. Robin Owen (Didcot, UK) – X-ray Crystallography: From Electrons in an Undulator to Electrons in a Crystal

10:30 Coffee

11:00 Social Science and Humanities

Prof. Dr. Peter Kroes (Delft, NL) – Ethical Implications and Social Consequences of New Technical Developments

13:00 Lunch

16:30 Coffee

17:00 Discussion Forum – CUI from the perspective of the PhDs

18:30 PhD Talks: Session 4

19:30 Feedback Forum – Time to discuss content and format of this Winter School

20:00 Dinner

Friday

07:30 Breakfast

08:00 PhD Talks: Session 5

10:00 Coffee

10:15 PhD Talks: Session 6

11:45 Lunch

13:15 Departure

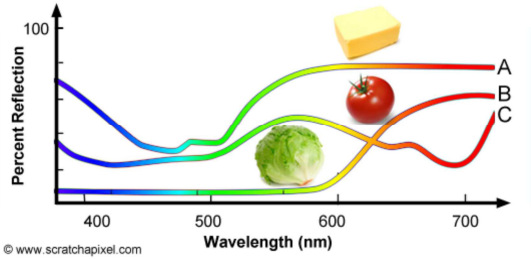
Lectures: Area A

Light Matter Interaction - Selected Topics in Photonics

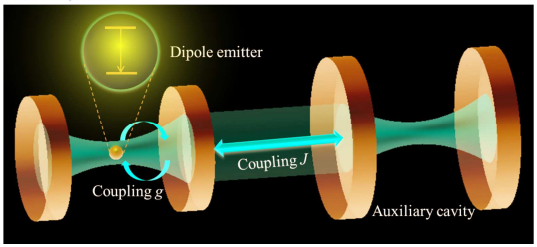
Prof. Dr. Jochen Küpper, Center for Free Electron Laser Science (Hamburg, DE)

In this lecture we will discuss fundamental concepts of matter interacting with light and, more broadly with electromagnetic waves in general. This includes basic effects such as the absorption and emission of light, the photoelectric effect, or the manipulation and control of molecules with electromagnetic fields.

We will discuss applications ranging from precision spectroscopy with optical light, over molecule-detection techniques and astronomic observations, to ultrafast diffractive x-ray imaging of matter. Furthermore, we will discuss how light allows to prepare samples for such investigations, through mechanical control or the triggering of dynamics.



Spectral reflectance curve of butter (A), tomato (B) and lettuce (C)

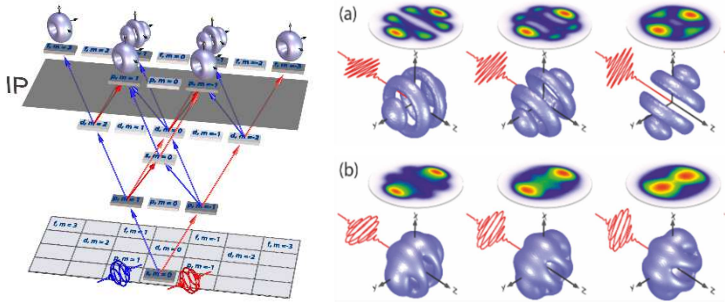


Single-photon single-emitter interactions (time-permitting, likely too advanced for the course…)

Coherent Control of Ultrafast Processes in Molecular Dynamics

Prof. Dr. Matthias Wollenhaupt, TU Kaiserslautern (DE)

Femtosecond spectroscopy is a tool to observe ultrafast molecular dynamics in the time domain. The active manipulation of quantum systems employing ultrafast pulse shaping techniques has emerged as a new research field termed coherent control. Specifically, in coherent control, shaped femtosecond laser pulses are used to steer the ultrafast light-induced dynamics of a quantum system from a given initial state to a predefined target state with high selectivity and high efficiency.



Left: physical mechanism of coherent control of multiphoton ionization by interference of multiple pathways using polarization-shaped femtosecond laser pulses, right: tomographic reconstruction of free electron wave packets using linearly (a) or elliptically (b) polarized laser pulses.

In the lectures, we will discuss the physical principles of coherent control by shaped femtosecond laser pulses. Initially, we consider the interaction of shaped laser pulses with matter in the perturbative regime to portray some established quantum control scenarios based on multi-path quantum interference. The focus of the lectures is on non-perturbative interactions of atoms and molecules in intense laser fields that enable new physical mechanisms to control the ensuing dynamics.

Lectures: Area B

Proteins - Structure and Function

Prof. Dr. Henning Tidow, Hamburg University (DE)

Proteins are the most versatile macromolecules in living systems and serve crucial functions in essentially all biological processes. They function as catalysts, transport and store other molecules such as oxygen, provide mechanical support and immune protection, generate movement, transmit nerve impulses, and control growth and differentiation.

As function of proteins is determined by their structure, structural biology is the key to understand the structure-function relationship of proteins. In my lecture, I will briefly introduce basic principles that determine the structure of proteins as well as experimental techniques that can be used to study protein structure. Selected examples will be used to illustrate the role of protein dynamics, conformational changes and protein-protein interactions in various physiological processes.

In the second lecture I will focus on membrane proteins and explain their special characteristics. Structure and function of different classes of integral membrane proteins will be introduced and discussed in relation to the biochemical/physiological processes they are involved in.

X-ray Crystallography: From Electrons in an Undulator to Electrons in a Crystal

Dr. Robin Owen, Diamond Light Source (Didcot, UK)

The fundamental aspects of macromolecular X-ray crystallography at synchrotrons and free electron lasers will be covered. This will range from a revision of the theory of diffraction and generation of X-rays at synchrotrons and XFELs, to review and discussion of the state-of-the art in instrumentation. Aspects such as beamline instrumentation, sample delivery and data analysis will be covered with, where possible, current research projects used as examples.

Lectures: Area C

Nanoporous Solids

Prof. Dr. Simone Mascotto, Hamburg University (DE)

A privileged strategy to improve many properties of inorganic materials is nanostructuring. In this respect, the introduction of nanoporosity is particularly desired for applications, such as heterogeneous catalysis, gas sensing or separation, where the interface between the fluid and the solid needs to be maximized. The porous structure ensures not only an easy access to the oxide grains within the pore walls, it also shortens the diffusion path lengths and, thus, fastens the kinetics of these processes.

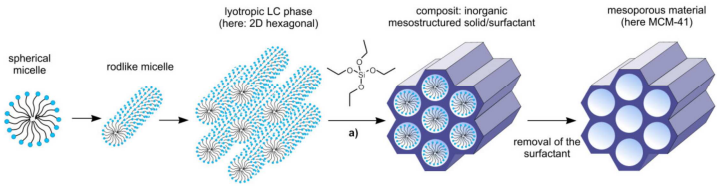


Fig. 1: Soft-templating approach for the synthesis of mesoporous SiO2[Chem. Rev.2007, 107, 2821]

These lectures will give an overview on the different synthesis strategies towards nanoporous solids, with major focus on softtemplating (Fig. 1). Here organic amphiphilic molecules (e.g. surfactants or block copolymers) organize in micelles and act as structure directing agents during hydrolysis and condensation reactions of the inorganic precursor. After elimination of the organic phase, a mesoporous material (pore width: 2-50 nm) is obtained. In addition different classes of nanoporous solids such as zeolites, MOFs, mesoporous silica and organosilica will be described giving particular attention to their potential industrial applications.

Fundamental Principles of Nanoparticle Formation

Dr. Jörg Polte, HU Berlin (DE)

Colloidal nanoparticles have attracted much attention due to their unique properties and promising applications. Synthetic procedures are known and have been investigated since Faraday's ground-breaking experiments about gold colloids more than 150 years ago.[1] In the past 25 years, the synthesis, characterization and application of colloidal nanoparticles turned into one of the most vivid research fields.[2]

In this regard, it is suprising that the actual nanoparticle formation processes remain a black box. In general, progress in synthetic procedures is achieved by trial and error approaches without having a precise idea of the underlying growth mechanisms. Simple questions of fundamental interest such as (i) "What is the principal growth mechanism?", (ii) "What determines the final particle size?" or (iii) "How do the different synthesis parameters affect the growth mechanism and therefore the final size or shape?" cannot be answered.

In the first lecture the common models to desribe particle formation are introduced and in the second lecture, the current experimental approaches for investigations of particle syntheses are presented. Furthermore, a detailed study for the most common gold nanoparticle synthesis - the Turkevich method- is presented. It provides answers to the three aforementioned questions. In fact, size control is already achieved for this specific synthesis.[6-8] However, the experimental approach, the gained mechanistic knowledge and the derived growth model are of general interest and can be transferred to several other synthetic procedures.

1) Faraday, M., Philosophical Transactions of the Royal Society of London, **1857**,147, 145
2) Xia, Y. et al., Angew. Chem. Int. Ed., **2009**,48, 1, 60

Social Science & Humanities

Ethical Implications and Social Consequences of New Technical Developments

Prof. Dr. Peter Kroes, Delft University of Technology (NL)

After a brief discussion of the notion of ethics, I will present an overview of different kinds of ethical issues related to science and technology. I will distinguish between moral issues with regard to (i) the products of science ("knowledge") and technology ("technical artefacts"), (ii) science and technology as social practices, and (iii) science and technology as specific kinds of problem-solving activities. All these different kinds of moral issues are involved in addressing the question: How to be a good scientist/engineer? I will argue that in dealing with this question we will have to distinguish between two different notions of goodness: goodness in the moral and in the methodological sense. In the second part I will focus on scientific integrity. We will discuss clear cases of manipulation of data that violate being a good scientist/engineer in both senses, but also a case in which it is not so clear whether the norms of being a good scientists/engineers were violated. I will also briefly address the question why issues about scientific integrity have become so prominently on the agenda of the scientific/technical community. Finally I will address a specific issue with regard scientific integrity that concerns PhD-students in particular, namely the role of Informed Consent in accepting to perform a PhD project. I will do this through a debate about the following Informed-Consent-Proposition:

Every PhD thesis supervisor has the moral duty to fully inform the PhD student about the broader context of his/her PhD project (aim, funding, possible applications, IP issues etc.) and every PhD student has the moral duty to inquire into the broader context of his/her PhD project?

PhD Workshops & Discussion Forum

PhD Workshops

The workshops offer the opportunity to meet with colleagues from related fields and discuss research projects in more detail. We do not want to impose any topics that should be discussed. We think more interesting discussion groups can be formed in a self-organized manner – you know best who is doing the most interesting research within CUI for you. Since this workshop – despite the title – should not be exclusively for PhDs try to catch one of the Postdocs or Speakers for your Session.

Posters will be provided in one of the seminar rooms to provide a location for the organization process. Write down your topic and leave some space for participants to register.

Discussion Forum

As CUI is running now for more than three years we want to continue the discussion on the research cluster from our point of view. Where can we benefit from its interdisciplinarity? Did we make progress in developing a common language across the borders of disciplines? What does all this mean in our daily lives as young researchers?

In order to give a large number of people the possibility to actively participate in the discussion we suggest to split up into smaller groups of 5 to 10 people. After half of the time we will meet again all together and one representative of each group will report the findings and we will open a podium discussion.

A paper with some guiding questions will be provided to facilitate the start of the discussion. Pick the two or three most interesting ones from the sheet to discuss about. You can also can discuss questions not on the sheet and present it later in the plenary part.

PhD Talks

Session 1 A

(Monday 17:30 – 19:30, chair: Markus Jakob)

- Malik Muhammad Abdullah – *Calculation of the X-ray Scattering Intensity from Nanocrystals Exposed to Spatially Inhomogeneous High-intensity Hard-X-ray Beams*
- Kai Bagschik – *Imaging of Magnetic Nanodots using X-ray Holographic Microscopy*
- Alexander Britz – *Ultrafast X-Ray Experiments with Extreme Signal Quality*
- Caroline Arnold – *The Influence of Nuclear Motion on Electronic Decoherence at Short Times*
- Lara Frenzel – *XPCS Studies of Complex Fluids*

Session 1 B

(Monday 17:30 – 19:30, chair: Maria Katsiaflaka)

- Julius Nitsche – *The Structure of the Calcium-ATPase from Arabidopsis Thaliana*
- Robin Schubert – *Reliably Distinguishing Protein Nanocrystals from Amorphous Precipitate by Means of Depolarized Dynamic Light Scattering*
- Aileen König – *Structure Function Relationship of the Leucine Rich Repeat Protein YopM of Pathogenic Yersinia*
- Yasser Almeida Hernandez – *Structural Studies of Rhomboid Proteases*
- Zeinab Eskandarian – *Plasma Membrane Calcium ATPase of Chaetomium Thermophilum*

Session 2 A

(Tuesday 08:30 – 10:30, chair: Peter Zalden)

- Bernhard Ruff – *Local Ionization of Ultracold Gases Induced by Femtosecond Laser Pulses*
- Neele Grenda – *Local Probes for Light-driven Intra-molecular Charge Transfer*
- Martin Ranke – *Laser-based THz-field Driven XUV Streak Camera for Time-resolved Measurements of Angular Energy Distribution of Electrons*
- Markus Jakob – *Molecules in Shaped THz (IR) Light Fields: Advancing Coherent Control in the Electronic Ground State*
- Emanuele Minutella – *Transient Absorption Spectroscopy on Colloidal Gold Nanoparticles*

Session 2 B

(Tuesday 08:30 – 10:30, chair: Christian Ziemann)

- Maria Katsiaflaka – *Synthesis of 2D MOFs by applying the Langmuir Schaefer Method*
- Mona Rafipoor – *Auger Recombination and Charge Transfer of CdSe/CdS Core/Shell Quantum Dot/Quantum Rods*
- Tobias Redder – *Gold Nanoparticle Growth*
- Robert Seher – *From Clusters to Nanocrystals: Investigation of Nucleation and Growth of Semiconductor Nanocrystals through use of a Continuous-Flow Device*
- Ramakrishna Vasireddi – *Microfluidic Devices for Ultrafast Structural Dynamics and Biological Applications*

Session 3 A

(Tuesday 19:00 – 20:00, chair: Alexander Britz)

- Alexander Achner – *Ionization and Dissociation Dynamics in 2-color Experiments*
- Michael Diez – *Ultrafast Spectroscopy of Functional Transition Metals*
- Daniel Riebesehl – *Investigation of Fast Dynamic Processes in Ultrathin Films excited with Ultrashort Magnetic Pulses*

Session 3 B

(Tuesday 19:00 – 20:00, chair: Aileen König)

- Stephanie Kesgin-Schäfer – *Incorporation of Unnatural Amino Acids in Transmembrane Proteins*
- Sebastian Fuchs – *Structural Analysis of Uba5 and its Binding Partners*
- John Joseph Doyle – *Photocages and Unnatural Amino Acids for Time Resolved Studies of Protein Reactions*

Session 4 A

(Thursday 18:30 – 19:30, chair: Kore Hasse)

- Markus Pfau – *High Harmonic Source with Monochromator for ICD-Experiments*
- Sadegh Bakhtiarzadeh – *Relativistic Electron Diffraction of Gas Phase Dynamics in Molecules*
- Fawad Karimi – *Following the Evolution of Interatomic Coulombic Decay (ICD) in Time Domain*

Session 4 B

(Thursday 18:30 – 19:30, chair: Alice Cantaluppi)

- Viktor Valmispild – *Magnetic Susceptibility in TM-Systems*
- Peter Zalden – *Terahertz-induced Switching in Chalcogenide Glasses for Novel Electronic Memory Devices*
- Helen Bieker – *Disentangling Water Cluster Beams*

Session 5 A

(Friday 08:00 – 10:00, chair: Helen Bieker)

- Kore Hasse – *Femtosecond Laser Structuring of Thin Disk Gain Materials*
- Masoud Mehrjoo – *Towards Single-shot Measurements of FEL Wavefronts*
- Anastasios Dimitriou – *THz-field-driven XUV Streak Camera for the Study of Femtosecond Electron Dynamics*
- Thomas Seine – *FEL-Application in Structural Biology*
- Sabine Botha – *Towards Time-resolved Serial Crystallography*

Session 5 B

(Friday 08:00 – 10:00, chair: Kai Bagschik)

- Joscha Reichert – *System-Bath Dynamics in Driven Environments*
- Christian Ziemann – *Bond-selective Excitation of Acetylene-d_1*
- Christian Gramsch – *Lehmann Representation of the Non-equilibrium Self-energy*
- Lars Thormann – *Structural Studies on the Dynamics of Membrane Proteins in the Crystalline and the Solution State*
- Jakob Benedikt Mietner – *Structural and Thermodynamic Studies on the Phase Behavior of Water in Ordered, Nanoporous Host Structures with Different Pore Sizes and Different Surface Polarities*

Session 6 A

(Friday 10:15 – 11:45, chair: Mona Rafipoor)

- Dina Sheyfer – *Structure and Dynamics of Cubic Hematite Nanoparticles*
- Vera Lebedeva – *Mechanical Properties of Freely Suspended PbS Nanosheets*
- Marina Mutas – *Fluorescence Lifetime Imaging of Gold Nanoclusters on/in Cells*
- Anastasia Karpulevich – *Colloidal Quantum Dots from the Position of Computer Modelling*

Session 6 B

(Friday 10:15 – 11:45, chair: Michael Diez)

- Alice Cantaluppi – *Stimulated Superconducting-like Properties in K_3C_{60} far above the Equilibrium Critical Temperature*
- Johannes Schurer – *Ultracold Quantum Chemistry*
- Niclas Luick – *Local Probing of Phase Correlations in a Strongly-interacting Two-dimensional Quantum Gas*
- Mohammad Vakili – *Ultrafast Reaction Kinetics in Microfluidic Geometries*

Location & Travel

Location

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Kapellenweg 2
79682 Todtmoos-Strick

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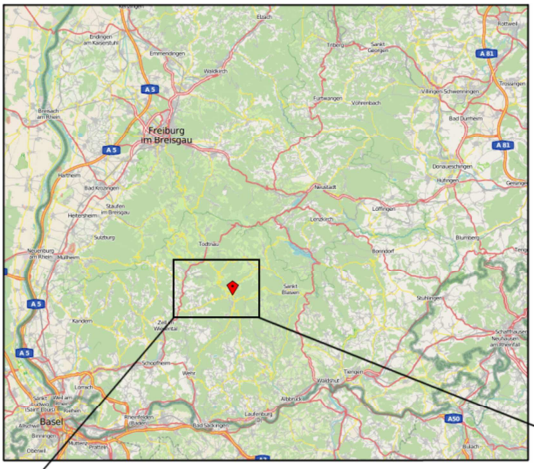
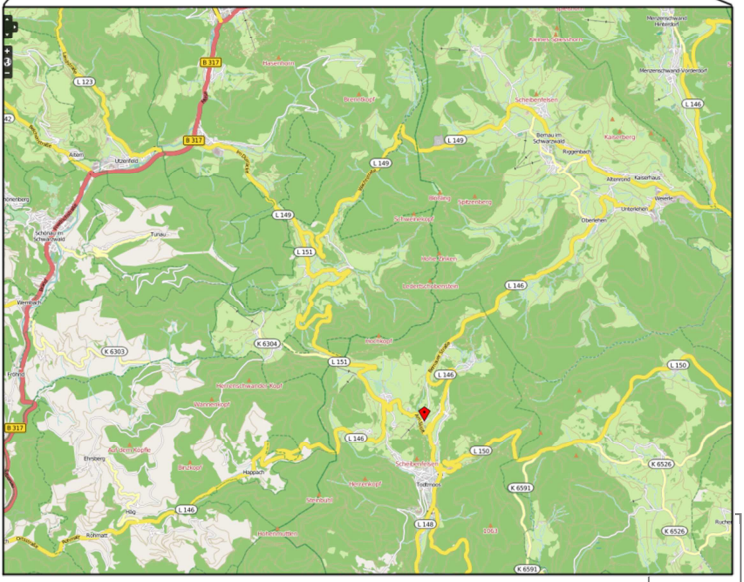
Email: info@hotel-roessle.de

Directions

By car via A5: Leave A5 at Freiburg Mitte and proceed towards Titisee and leave Freiburg. You will travel on B31 until Kirchzarten/Todtnau is indicated. Leave here and proceed to Todtnau. There turn right in the direction of Basel/Todtmoos. After 4 km turn left towards Todtmoos. After crossing the top of the pass you will find yourself in the district Todtmoos-Weg. Follow the street until you reach Todtmoos-Strick. The distance from Freiburg Mitte is about 50 km and about 1 hour of travel.

***By car via A81*:** Leave A81 in Donaueschingen und proceed in the direction of Freiburg and Titisee-Neustadt. There turn right and follow the road towards Basel/Todtnau. In Bärental go on B500 towards Schluchsee/Waldshut. When you enter Schluchsee turn immediately right. Go on via Menzenschwand to Bernau. There turn left, pass through the village and go on to Todtmoos. To find the district Todtmoos-Strick go on a bit further in the direction of Freiburg. Starting from Donaueschingen it takes 90 minutes to reach to Hotel (80 km).





By Train: The nearest train station is Seebrugg, which you can reach best via Freiburg i. B. From Seebrugg there is a bus service available. It takes about 1.5 hours and leaves every 2 hours. By Taxi it should take only half an hour to get from Seebrugg to Todtmoos.

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Notes