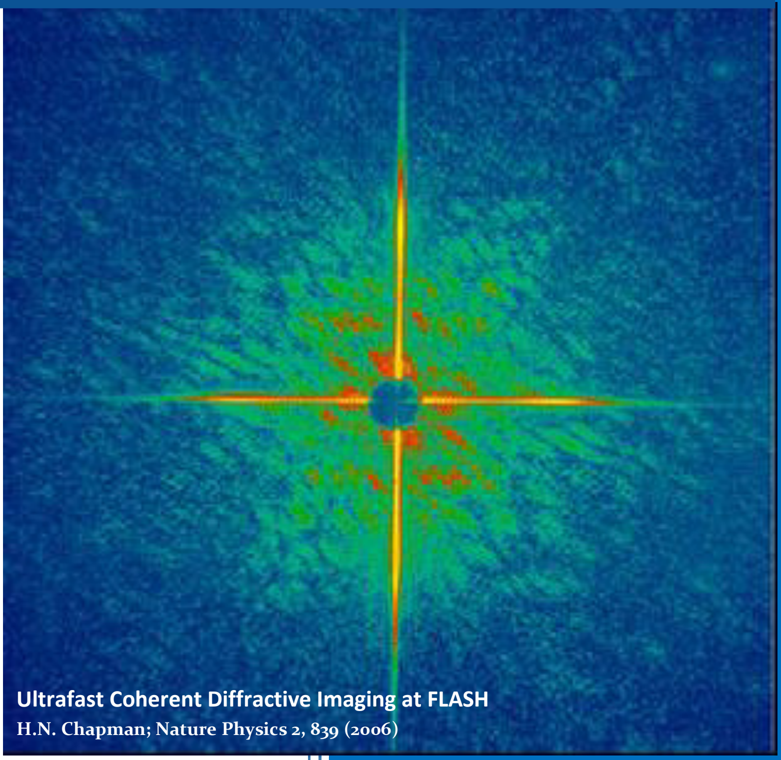
CUI

THE HAMBURG CENTRE
FOR ULTRAFAST IMAGING

2013

Winter School



Ultrafast Coherent Diffractive Imaging at FLASH
H.N. Chapman; Nature Physics 2, 839 (2006)

Obergurgl (Austria)

02.12 – 05.12.2013

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 are 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.

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Timetable and program

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16:15 **Dr. Gerd Schneider**
X-ray and electron microscopy (Part 1)

18:00 **Ph.D. talks**
Kai Bagschik
Johannes Schurer
Pankaj Kumar Mishra

20:00 **Dinner**

21:15 **Poster Session 1**

Tuesday, 03.12.2013

07:30 **Breakfast**

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X-ray and electron microscopy (Part 2)

10:15 **Dr. Juliette Simonet**
Ultracold quantum gases (Part1)

16:15 **Dr. Leonard Müller**
Ultrafast dynamics of magnetic domain Structures probed by coherent Free-Electron Laser light

18:00 **Ph.D. talks**
Sabrina Zinn
Robin Schubert

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08:30 **Dr. Juliette Simonet**
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10:15 **Prof. Dr. Sonia Melandri**
Microwave spectroscopy of biomolecules And their weakly bound molecular complexes (Part 1)

16:15 **Prof. Dr. Sergej O. Demokritov**
Magnetic excitation in nanostructures (Part 1)

18:00 **Ph.D. talks**
Robert Seher
Yudong Yang

20:00 **Dinner**

21:15 **Poster Session 2**

Thursday, 05.12.2013

07:30 **Breakfast**

08:30 **Prof. Dr. Sonia Melandri**
Microwave spectroscopy of biomolecules And their weakly bound molecular complexes (Part 2)

16:15 **Prof. Dr. Sergej O. Demokritov**
Magnetic excitation in nanostructures (Part 2)

18:00 **Ph.D. talks**
Malte Behrmann
Bernhard Ruff

20:00 **Dinner**

Ph.D. student posters

Bastian Deppe (Institute for Laser Physics, DESY, A)
CW laser induced alignment of molecules

Neele Grenda (University of Hamburg, DynamiX, A)
Local probes for light-driven intra-molecular charge transfer

Jens Kienitz (Centre for Free-Electron Laser Science, DESY, A)
Rotational dynamics, alignment and orientation of state-selected OCS molecules

Vijay Pal Singh (Centre for Optical Quantum Technologies, DESY, A)
Noise correlations and superfluid behavior of two-dimensional Bose gases

Thomas Kierspel (Centre for Free-Electron Laser Science, DESY, A)
Molecular state selection and species separation by deflection

Muhammed Saqib (Centre for Free-Electron Laser Science, DESY, A)
Multiwavelength anomalous Diffraction at high X-Ray intensity

Robert Büchner (Institute for Laser Physics, DESY, A)
Orbital physics with ultracold atoms in higher Bands of an optical lattice

Franziska Krawack (University Medical Center Hamburg-Eppendorf, Institute of Medical Microbiology, B)
Investigation & visualization of the Yersinia translocation pore

Salah Awel (Centre for Free-Electron Laser Science, DESY, B)
An optical pipeline for femtosecond diffractive imaging

Carsten Thönnißen (Institute of Applied Physics, University of Hamburg, C)
Imaging Magnetic Nanodots with Soft X-Ray Holographic Microscopy

Christian Swoboda (Institute of Applied Physics, University of Hamburg, C)
Dynamic coupling of magnetic resonance modes in pairs of mesoscopic rectangles

Benedikt Mietner (Institute of Inorganic and Applied Chemistry, University of Hamburg, C)
Structural and thermodynamic studies on the phase behavior of water in ordered, nano- and mesoporous host structures with different surface polarities

Tobias Redder (Institute for Physical Chemistry, University of Hamburg, C)
X-ray diffraction of gold nanoparticles in a Free Liquid Jet

Dina Sheyfer (Coherent X-ray Scattering Group, DESY, C)
Soft colloidal spheres studied by coherent X-rays

Vera Paulava (Institute for Physical Chemistry, University of Hamburg, C)
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Ph.D. student talks

Yudong Yang (Centre for Free-Electron Laser Science, DESY, A)
Techniques for isolated attosecond pulse generation

Bernhard Ruff (University of Hamburg, DynamiX, A)
Coherence and decoherence of electrons emerging from Bose-Einstein condensate

Johannes Schurer (Centre for Optical Quantum Technologies, DESY, A)
Quantum many-body simulations of the hybrid atom-ion system confined in 1D

Malte Behrmann (Institute for Laser Physics, DESY; A)

Pankaj Kumar Mishra (Centre for Free-Electron Laser Science, DESY, A)
Ultrafast energy transfer to liquid water by sub-picosecond high-intensity terahertz pulses

Sabrina Zinn (Centre for Free-Electron Laser Science, DESY, B)
Broadband Microwave Spectroscopy of Biologically Relevant Complexes in the Gas Phase

Robin Schubert (Institute of Biochemistry & Molecular Biology, University of Hamburg, B)
Production and scoring of micro and nano protein crystals for analysis at synchrotron and X-ray free-electron laser radiation sources

Robert Seher (Institute for Physical Chemistry, University of Hamburg, C)
Continuous Flow Device for in-situ Investigation of Semiconductor Nanoparticle Nucleation and Growth

Kai Bagschik (Institute of Applied Physics, University of Hamburg, C)
High Resolution Magnetic Imaging with Soft X-Ray Holographic Microscopy

Magnetic Excitation in Nanostructures

S. O. Demokritov

University of Muenster, Corrensstrasse 2-4, 48149 Muenster, Germany

The concept of dynamic magnetic excitation of unconfined magnetic media called spin waves was introduced by Bloch in 1930. A spin wave represents a wave of spin precession propagating in a magnetically ordered medium.

Being of great importance for basic research of magnetically ordered systems, spin waves play a decisive role for technical applications as well. In fact, since spin waves are eigen-modes of magnetic media, the dynamics of magnetization can be nicely analyzed based on the spin-wave approach. Knowing the properties of spin waves, one can obtain a vital information on the temporal response of the magnetic media to pulses of the magnetic field or microwave radiation. Apparently this knowledge is basis for the creation of new magnetic sensors, memory elements, and re-programmable magnetic logic.

The history of the magnetic conception is inseparably linked with the reduction of the dimensions. Being first introduced for bulk media, spin waves in magnetic films have attracted enormous interest 60s and 70s of the last century. It was found that the confinement caused by the finite thickness of a film results in a variety of new effects and even new types of spin waves. The so-called surface spin waves were introduced theoretically by Damon and Eshbach in 1961 and then observed experimentally Grunberg and Metawe in 1977. Therefore, it is not surprising that the interest to spin waves in films was a forerunner of a wide application of magnetic films in the information technology.

Magnetization dynamics in laterally confined magnetic nanostructures is in the focus of the current research. Nowadays, one-dimensional and zero-dimensional magnetic nanoobjects are investigated very actively. This trend is closely connected with the recent developments in the field of high-density magnetic storage and miniature magnetic sensors. Another advantage of magnetic nanostructures is that in systems with small dimensions very dense charge- and spin-currents can be produced. Interacting with localized magnetic moments these currents can bring about completely new physical phenomena

In my lectures I will first focused on the physical effects associated with the confinement and address the issue of laterally quantized magnetic excitation. Then I will focus on the interplay between spin transport and magnetization. The effect of spin-polarized electric current as well as of pure spin current on magnetic dynamics in nanostructures will be discussed. Finally, several specific devices as spin-torque nano-osccilator and spin-Hall nanooscillator will be considered.

Microwave spectroscopy of biomolecules and their weakly bound molecular complexes

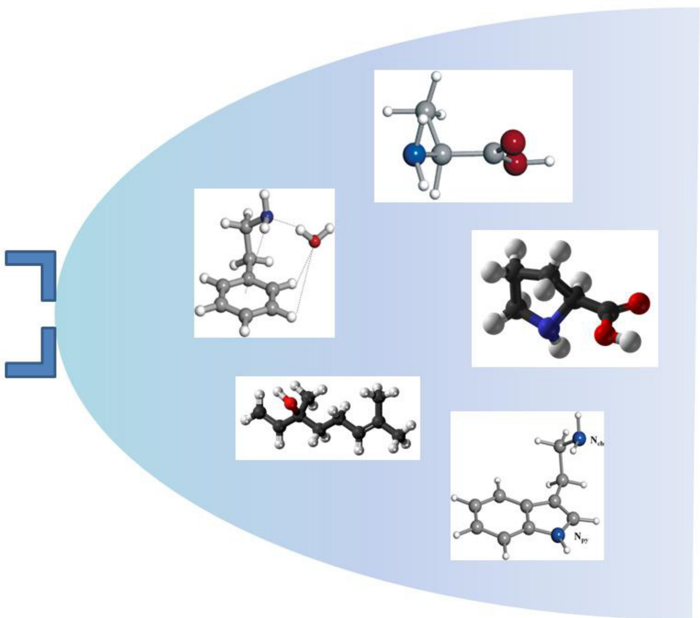
S. Melandri

"G. Ciamician" Department of Chemistry, University of Bologna, Via Selmi 2, I-40126 Bologna, Italy.

Biomolecules are characterized by an extreme conformational flexibility originating from multiple torsional degrees of freedom, which make folding and functionality possible.
While the topology of the molecule is determined by covalent forces, the conformational space of such systems is generally shaped by non bonding interactions occurring within the molecule or with the surroundings. The high number of low energy conformations and the presence of large amplitude motions taking place through shallow potential energy surfaces are peculiar of these flexible molecules and their weakly bound molecular complexes.

Rotational spectroscopy of biomolecules isolated in the gas phase in the conditions of a supersonic expansion gives very detailed structural and dynamical information on their intrinsic properties. These properties in turn can be directly compared to the outcome of high level *ab initio* calculations which are used to rationalize the results.

Chosen examples will be given of rotational spectroscopy of biomolecules and small molecular complexes studied in the isolated conditions of a free jet expansion. They include: the adrenergic neurotransmitter (tyramine, serotonin, amphetamine and the ephedras), aminoacids, drugs, anesthetics, odorants and model systems. We will show how non-bonding interactions compete to shape their conformational space and how these interactions can be changed drastically through substitution of even a single atom. Moreover complexation can have influence on the flexibility of molecules changing the nature of the interactions and thus the shape of the conformational surface.



Ultrafast dynamics of magnetic domain structures probed by coherent Free-Electron Laser light

Leonard Müller

The free-electron laser (FEL) sources FLASH in Hamburg, LCLS at Stanford and FERMI in Trieste provide XUV to soft and even hard (LCLS) x-ray radiation with unprecedented parameters in terms of ultrashort pulse length, high photon flux, and coherence. These properties make FELs ideal tools for studying ultrafast dynamics in matter on a previously inaccessible level. Combining the high time resolution with the element selectivity, the spatial resolving power of x-rays, high photon flux, and excellent coherence properties FEL sources promise a pivotal step forward, especially in the investigation of ultrafast phenomena on nanometer length scales. One example, being in focus here, is ultrafast demagnetization [1] which is acting on time scales of a few 100 fs, which are not accessible at standard synchrotron radiation sources. Results obtained in the field of magnetism research at FEL sources will be reviewed, including pioneering experiments at FLASH demonstrating the feasibility of magnetic scattering at FELs [2, 3] (Fig. 1 a), an ultrafast pump–probe scattering experiment [4] as well as the first FEL magnetic imaging experiments at LCLS [5] and more recently at FERMI (Fig. 1 b, c).

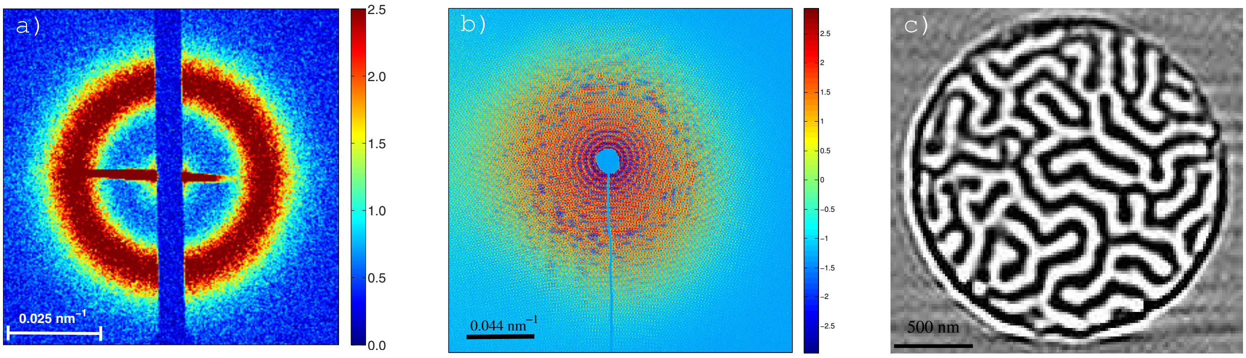


FIG. 1. a) First resonant magnetic small-angle scattering pattern taken at an FEL (FLASH) using a single pulse of 30 fs duration at the cobalt M-edge at 59.6 eV. b) Hologram of a magnetic domain system taken at the cobalt M-edge at FERMI. c) Reconstruction of the real space domain structure.

[1] E. Beaurepaire, J.-C. Merle, A. Daunois, and J.-Y. Bigot, Phys. Rev. Lett. **76**, 4250 (1996).

[2] C. Gutt, L. M. Stadler, S. Streit-Nierobisch, A. P. Mancuso, A. Schropp, B. Pfau, C. M. Günther, R. Könnecke, J. Gulden, B. Reime, et al., Phys. Rev. B **79**, 212406 (2009).

[3] C. Gutt, S. Streit-Nierobisch, L.-M. Stadler, B. Pfau, C. M. Günther, R. Könnecke, R. Frömter, A. Kobs, D. Stickler, H. P. Oepen, et al., Phys. Rev. B **81**, 100401(R) (2010).

[4] B. Pfau, S. Schaffert, L. Müller, C. Gutt, A. Al-Shemmary, F. Büttner, R. Delauny, S. Düsterer, S. Flewett, R. Frömter, et al., Nat. Commun. **3**, 1100 (2012).

[5] T. Wang, D. Zhu, B. Wu, C. Graves, S. Schaffert, T. Rander, L. Müller, B. Vodungbo, C. Baumier, D. P. Bernstein, et al., Phys. Rev. Lett. **108**, 267403 (2012).

X-ray and electron microscopy

Gerd Schneider
BESSY m.b.H., Albert-Einstein-Str. 15, 12489 Berlin, Germany

Biological cells are highly complex nanoscale three-dimensional objects. Imaging cells with high spatial resolution requires advanced microscopy techniques. Electron microscopy was the first technique which showed cellular features below the light microscopy level. Its high spatial resolution is due to the very short de Broglie wavelengths of fast electrons. The original form of electron microscopy, Transmission electron microscopy (TEM) involves a high voltage electron beam emitted by a cathode and formed by magnetic lenses. The electron beam is partially transmitted through very thin specimen and carries information about the object structure. The spatial variation of the transmitted electron beam is then magnified by a series of magnetic lenses until it is recorded on a CCD detector screen. Several decades our understanding of cells was formed by TEM imaging of dehydrated, plastic embedded, staining with heavy metals and finally thin-sectioned samples. All these processing steps involve potential artifacts in the cellular structure.

Mainly in the last two decades cryo electron microscopy became a new “gold standard” for visualizing the cellular ultrastructure of frozen-hydrated samples near the native state. Cryo TEM overcomes all limitations of conventional TEM preparations except it still requires thin samples which is caused by the short mean free path length for inelastic scattering of the fast electrons in matter. In combination with tomography, cryo EM has delivered 3-D views of cellular structures with a few nanometer resolution. Its main limitation comes from radiation damage which requires low-dose imaging.

Light microscopy on the other hand is an established technique in biophysical investigations of cells, whereas cryo EM and especially cryo X-ray microscopy are relatively new methods. X-ray microscopy enables imaging of whole hydrated. Conventional fluorescence images are diffraction-limited to ~200 nm, whereas current x-ray images can achieve a ten-fold improvement in resolution, namely ~20 nm. The interaction of x-rays is element specific, therefore, x-ray nano-tomography can be used to quantify the packing density of organic material. However, different proteins or molecular structures cannot be distinguished directly in x-ray microscope images. This problem is solved by the availability of specific fluorescent probes detectable by fluorescence microscopy. Thus all these imaging modalities are complementary. Since fluorescence and x-ray microscopy permit analysis of whole cells, it is possible to investigate the same cell in both microscopes. These correlative studies are ideally suited to x-ray microscopy because of its ability to image cells in 3-D.

In the lecture, basic concepts of electron and X-ray microscopy will be presented and examples for their scientific applications will be shown. In addition, the current status as well as future aspects of x-ray microscopy at 3rd generation electron storage rings and the Free Electron Lasers with their fs-pulses will be discussed.

Ultracold Quantum Gases

Juliette Simonet
Institute for Laser Physik – University of Hamburg, Germany

Research on ultra-cold atoms is a very rich area of investigation, where different fields of fundamental research merge, such as atomic, condensed-matter and many-body physics. The first realization of a Bose-Einstein condensate (BEC) has been observed almost simultaneously in 1995 by three groups working with different alkali atoms (Rb, Na, Li). Only few years later, the first degenerate Fermi gases were experimentally realized.

The first generation of experiments on those quantum objects revealed that their behavior is described by a macroscopic wave-function governed by a nonlinear Schrödinger equation. Most properties of weakly-interacting Bose-Einstein condensates in 3D were investigated in great details. Coherence properties and quantized vortices, providing a striking evidence for the superfluidity of Bose-Einstein condensates, are well described in a mean-field approach.

Within the last thirty years, research efforts in this field are undergoing a continuous expansion. The precise control of atomic interactions, taking advantage of Feshbach resonances in an external magnetic field, paved the way towards regimes of strong correlations described by complex many-body theories.

Such strongly correlated regimes can also be reached in optical lattices produced by far detuned standing waves of laser light. The precise control on the trapping potentials and the detailed description of the atomic interactions allows emulating a model Hamiltonian. Reference Hamiltonians were proposed and extensively studied in the field of condensed matter, for which numerical simulation is impossible. As a consequence ultracold gases constitute a unique tool to investigate open problems from condensed matter, via analogous simulation as initially proposed by Feynman.

In this lecture, I will first briefly review the experimental techniques used to realize and to probe degenerate ultracold gases. The second part concentrates on the impact of tunable interactions either in a BEC or in a Fermi gas. Finally the challenges and goals of the experimental platforms including optical lattices will be discussed.

Introduction to ultrafast multidimensional optical spectroscopy

Valentyn I. Prokhorenko

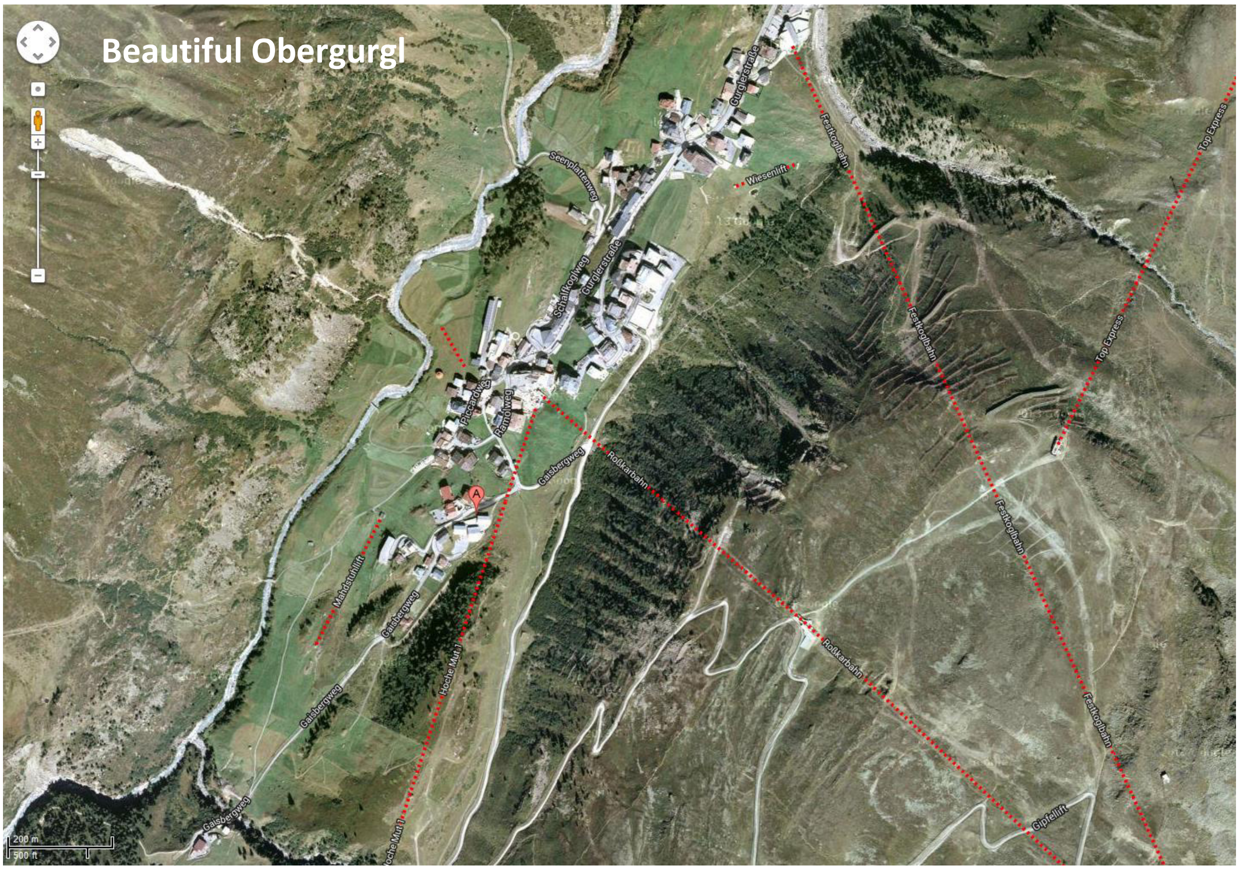
Max Planck Institute for the Structure and Dynamics of Matter
Center for Free Electron Laser Science CFEL
University of Hamburg, 22607 Hamburg, Germany
valentyn.prokhorenko@mpsd.mpg.de

Abstract

In the past decade, multi-dimensional optical spectroscopy (MDS) has become an invaluable scientific tool for the studying of ultrafast processes occurring in matter in sub-picosecond and femtosecond time scales. On the other hand, the structural organization of investigated system can also be recovered from so-called two-dimensional spectra (2D) (analogous to NMR), which has been successfully demonstrated in numerous 2D-IR experiments. Thus, MDS can also be viewed as some kind of "imaging technique"; however, the spatial resolution is limited by the size of sub-units forming an object (e.g. amino acids in a protein backbone).

In this lecture we will consider, starting from the very basic level, the theoretical principles of MDS, paying most attention to spectroscopies based on coherent properties of light-matter interaction (photon echo). In the second part we will review existing techniques and methods for acquiring multi- (basically two-) dimensional spectra in the optical range covering IR, VIS and very recent developments for the UV-range, as well as treatment techniques. The latest developments in this field, so-called coherently-controlled 2D-spectroscopy, will be also outlined. The last part of the lecture will be devoted to achievements in MDS and illustrated by latest results of 2D-VIS and UV spectroscopies.

Location


Beautiful Obergurgl
Wiesenlift
Top Express
Festkoglbahn
Roßkarbahn
Gaisbergweg
Gipfellift

LEGENDE / LEGEND

6er-/8er-Kabinenbahn / 6-seater/8-seater gondola	6er-Sesselbahn / 6-seater chairlift	4er-Sesselbahn/-lift / 4-seater chairlift	Schlepplift / T-bar lift
Tellerlift / Button lift	Seillift / Ski tow	Förderband / Magic carpet	leichte Piste / easy slope
mittelschwere Piste / intermediate slope	schwere Piste / difficult slope	Skiroute / Ski route	Rodelbahn / Tobbogan run
Winterwanderweg / Winter hiking trail	Langlaufloipe / Cross country ski trail	Beleuchtung / Floodlit pistes	Restaurant / Schirmbar / Restaurant / Open air bar
Funpark / Funpark	Geschwindigkeitsmessstrecke / Speed measurement	Permanente Rennstrecke / Permanent race track	Aussichtspunkt / Vantage point
Ruhezone / Chill-out Zone / Chill-out zone	Wildtiersafari Zauberwald / Magic forest wild animal safari	Eislaufplatz / Ice skating	Skibushaltestelle / Ski bus stop
Sammelplatz Schischule / Ski school's meeting place	Erste Hilfe / Arzt / First aid / doctor	Ötztal Information / Ötztal Information	Parkplatz / Parking lot
Wintersperre Timmelsjoch / Winter lock at Timmelsjoch	Hubschrauberlandeplatz / Helicopter landing place	Speicherteich Beschneiung / Reservoir snow-making facil	

Bright & Visionary

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