



The Hamburg Centre for Ultrafast Imaging
International Symposium 2015

Hamburg
Campus Bahrenfeld, CFEL
November 11 – 12



EMBL



The Hamburg Centre for Ultrafast Imaging

International Symposium 2015

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The Hamburg Centre for Ultrafast Imaging

International Symposium 2015

Programme

Wednesday, November 11, 2015

9:30 am.	Registration/Coffee
10:30 am.	Odelius, Michael <i>Theoretical simulations enabling insight into solution dynamics and electronic structure from core-level spectroscopy</i>
11:30 am.	Lunch Break
1:00 pm.	Lindenberg, Aaron <i>Ultrafast electric-field-driven processes in materials</i>
2:00 pm.	Verstraete, Frank <i>Entanglement matters: from Bell states to quantum tensor networks</i>
3:00 pm.	Coffee Break
3:30 pm.	Cirac, Ignacio (Prize Talk) <i>New frontiers in quantum optics and many-body physics</i>

Thursday, November 12, 2015

9:30 am.	Wilmot, Carrie <i>MauG catalysis: a tale of ferryl iron, radicals and long distance hopping</i>
10:30 am.	Quinn, Susan <i>Monitoring one-electron photo-oxidation of guanine in DNA in solution and in crystals using transient infrared spectroscopy</i>
11:30 am.	Lunch Break
1:00 pm.	Marrows, Christopher <i>Thermal fluctuations and freezing in artificial spin ice: X-ray photon correlation spectroscopy</i>
2:00 pm.	Manna, Liberato <i>Chemical and structural transformations in nanocrystals by ion exchange</i>
3:00 pm.	Coffee Break
3:30 pm.	Petterson, Lars <i>Water – a tale of two liquids</i>
4:30 pm.	Champagne Reception
5:00 pm.	Hamburg Prize for Theoretical Physics (Prize Session)

Hamburg Prize for Theoretical Physics 2015



Award Ceremony, November 12

5:00 pm

Welcome Address

Petra Herz

Chairwomen of the Executive Board, Joachim Herz Stiftung

Welcome Address

Katharina Fegebank

Second Mayor and Senator for Science and Research of Hamburg

Interview

Ralf Krauter

Science journalist

Prof. Klaus Sengstock

Spokesperson of The Hamburg Centre for Ultrafast imaging (CUI)

Dr. Jörg Maxton-Küchenmeister

Director Program Area Science, Joachim Herz Stiftung

Laudatory Speech

Prof. Eugene Polzik

Niels Bohr Institute, University of Copenhagen

Interview

Ralf Krauter,

Prof. Ignacio Cirac

Presentation of the Award to

Prof. Ignacio Cirac



Location, Contact and Directions

Location

Campus Bahrenfeld

Notkestraße 85 (Main Entrance)/Luruper Chaussee 149 (Side Entrance)

Building 99 (CFEL), Foyer Seminar-room I - III

Contact

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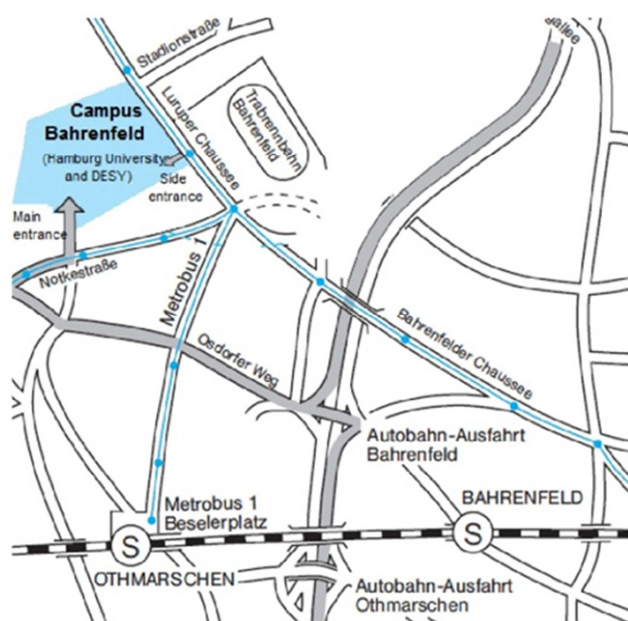
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Directions:



By train: to Hamburg-Altona station, then continue by taxi (travelling time ~15min) or take a bus (see below).

By bus: To reach the side gate (recommended), take bus line 2 (direction Schenefeld Mitte) from Altona train station and get off at "Luruper Chaussee/DESY", travelling time ~20min.

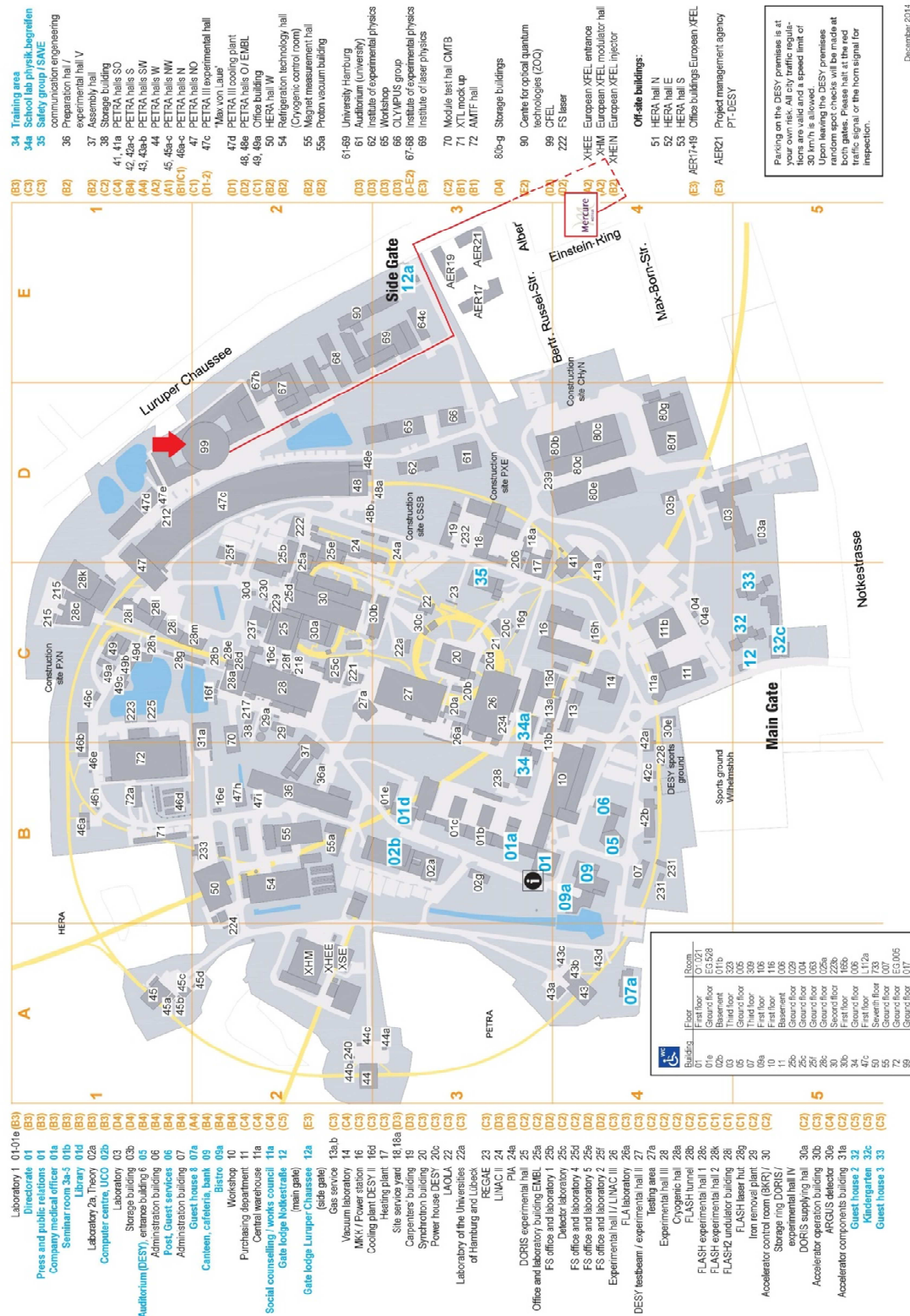
From train station "S-Bahn Othmarschen", take bus line 1 (direction "Schenefelder Holt") directly to the main entrance of the campus (bus stop "Zum Hünengrab/DESY"), traveling time ~25 min.

By plane: The campus can be reached from Hamburg airport by taxi in ~30min. Alternatively, take suburban train S1 to Altona or Othmarschen (~40min, direct train) and a bus from there (see above).

The Hamburg Centre for Ultrafast Imaging

International Symposium 2015

Campus Map



Location, contact and directions

December 2014

List of Invited Speakers

J. Ignacio Cirac (Max-Planck-Institut für Quantenoptik, München)

New frontiers in quantum optics and many-body physics

Aaron Lindenberg (Stanford University, SLAC National Accelerator Laboratory, Stanford)

Ultrafast electric-field-driven processes in materials

Liberator Manna (Istituto Italiano di Tecnologia, Genoa)

Chemical and structural transformations in nanocrystals by ion exchange

Christopher Marrows (University of Leeds, Leeds)

Thermal Fluctuations and Freezing in Artificial Spin Ice: X-ray Photon Correlation Spectroscopy

Michael Odelius (Stockholms universitet, Stockholm)

Theoretical simulations enabling insight into solution dynamics and electronic structure from core-level spectroscopy

Lars Pettersson (Stockholms universitet, Stockholm)

Water – a tale of two liquids

Susan Quinn (University College Dublin, Dublin)

Monitoring one-electron photo-oxidation of guanine in DNA in solution and in crystals using transient infrared spectroscopy

Frank Verstraete (Universität Wien, Wien)

Entanglement matters: from bell states to quantum tensor networks

Carrie Wilmot (University of Minnesota, Minneapolis)

MauG catalysis: a tale of ferryl iron, radicals and long distance hopping

Speakers' Abstracts

Aaron Lindenberg (Stanford University, SLAC National Accelerator Laboratory, Stanford)

Ultrafast electric-field-driven processes in materials

Novel characterization techniques developed over the past decade or so have revolutionized our ability to visualize the elementary processes that determine the functional properties of materials. The overarching challenge here is that the relevant time-scales and length-scales for these processes are typically 10-13 seconds (100 femtoseconds) and 10-10 m (1 Å) such that our views of how a material functions are often blurred out in time or in space. In this talk I will describe recent experiments utilizing femtosecond x-ray and optical pulses as a means of probing the dynamics of materials, in particular focusing on electric-field-driven processes in next generation materials for information processing. We carry out these experiments in electrode-less geometries using single-optical-cycle terahertz frequency light pulses as an all-optical bias. I will focus in detail in this talk on two broad examples: (1) I will describe experiments probing electric field-driven structural rearrangements in ferroelectric thin films, using femtosecond x-ray pulses (as well as nonlinear optical techniques) to resolve atomic-scale changes within the unit cell and the dynamics of the ferroelectric polarization. (2) I will describe experiments capturing the first steps in field-driven switching in phase-change memory materials, focusing on both the ultrafast electronic and structural changes that accompany the amorphous-to-crystalline transition

Christopher Marrows (University of Leeds, Leeds)

Thermal Fluctuations and Freezing in Artificial Spin Ice: X-ray Photon Correlation Spectroscopy

S.A. MORLEY¹, A. STEIN², M.C. ROSAMOND³, D.A. ALBA VENERO⁴, S. RILEY³, P. STEADMAN⁵, S. LANGRIDGE⁴ and C.H. MARROWS¹

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Artificial spin ices are manifestations of toy statistical mechanical models such as the square ice model studied in the 1960s [1,2]. State-of-the-art lithography of magnetic nanostructures allows the fabrication of so-called 'designer matter' where the macrospin of magnetic nanoislands can be mapped to the spins in this class of Ising-like models [3], allowing experimental realisations of these models. In initial studies of such systems, magnetostatically interacting arrays of these nanoislands were relaxed into low energy states through ac demagnetisation processes [4]. Whilst revealing the expected extensive degeneracy, this process needs to be described by an effective thermodynamics [5], since the islands moments are frozen in place and the system is athermal.

Here we report on thermally-induced dynamics of artificial spin ices formed from magnetic nanoelements whose lateral size is small enough that the energy barrier (proportional to island volume) to reversal is low enough with respect to $k_B T$ that thermal fluctuations take place at room temperature: the macrospin system is able to fluctuate and equilibrate [6,7]. The sizes of the NiFe islands in this study are $\approx 30 \text{ nm} \times 75 \text{ nm}$ and 8 nm thick, much smaller than those which can be

imaged with most current magnetic microscopy techniques. We have therefore turned to the use of resonant magnetic soft x-ray photon correlation spectroscopy (XPCS) to observe the time-time autocorrelations of the thermally induced magnetic fluctuations in this system [8,9].

In XPCS, a small part of the sample is illuminated coherently through a 10 micrometer pinhole. The resulting Bragg spots have speckle that can be imaged on a CCD camera. Since the photon energy is tuned to the Fe L_3 edge, part of the scattering is sensitive to the magnetic configuration of the illuminated array. As the sample's magnetic configuration varies with time, so do the details of the speckle pattern. This allows us to extract the island relaxation time τ as a function of interisland coupling and temperature.

At 180 K the sample is frozen and displays no dynamics on the measurement timescale of several hours, but displays increasingly fast dynamics up to 250 K, whereas at 295 K the fluctuations are too fast to measure within our CCD camera's data acquisition time of 40 ms. Between these temperatures the temperature dependence of can be fitted by a Vogel-Fulcher law, implying collective freezing of the fluctuations. We measure a stretching exponent close to unity for weakly interacting islands (556 nm lattice constant), describing diffusive-like behaviour, and an exponent larger than unity for strongly interacting arrays (280 nm lattice constant), indicating more coupled/jammed dynamics due to the designed-in frustration.

Acknowledgments

This work was supported by the EPSRC (grant numbers EP/J021482/1 and EP/I000933/1), STFC, and the Diamond Light Source. Research carried out in part at the Center for Functional Nanomaterials, Brookhaven National Laboratory, which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886. We thank S. S. Dhesi for the loan of the CCD camera.

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Lars Pettersson (Stockholms universitet, Stockholm)

Water – a tale of two liquids

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I will discuss recent experimental and simulation data of liquid water and the picture of fluctuations between high-density (HDL) and low-density (LDL) liquid this has led to [1,2]. Such a two-liquid scenario would explain many anomalous properties, e.g., density maximum, heat capacity and isothermal compressibility minima, but no direct connection has been found to simulations of ambient water. Here I will discuss the temperature dependence in the O-O pair-distribution function at intermediate range ($< 18 \text{ \AA}$), which has recently been measured with good statistics [3], as well as implications for our understanding of structure and dynamics in water.

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Michael Odelius (Stockholms universitet, Stockholm)

Theoretical simulations enabling insight into solution dynamics and electronic structure from core-level spectroscopy

The challenge for a theoretically supported interpretation of core-level spectra both consists in faithfully simulating the spectroscopic process and in creating realistic models of the system. Liquid solutions require treatment of finite temperature effects and dynamical sampling and a balance description of local and long-range interactions. For this purpose density functional theory (DFT) in combination with molecular dynamics simulations can be used to sample relevant configurations and study dynamics. For the spectrum simulations, we often have to resort to high-level quantum chemistry, beyond DFT, to capture the correct physics and for the interpretation of high-resolution data. In the presentation, I discuss solution studies with photo-electron spectroscopy [1] and resonant inelastic X-ray scattering [2-4] giving detailed information on solute-solvent hydrogen bonding.

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Susan Quinn (University College Dublin, Dublin)

Monitoring one-electron photo-oxidation of guanine in DNA in solution and in crystals using transient infrared spectroscopy

Knowing the mechanism and dynamics of phot-induced DNA damage is critically important for our understanding of diseases associated with UV-irradiation as well as the development of photosensitised DNA-directed therapies. With photosensitisers, guanine oxidation is often the ultimate site of damage, a process which may be initiated by its one-electron photo-oxidation. The precise dynamics of this process are expected to be sensitive to both the location and the precise orientation of the photosensitiser on the DNA, features which are difficult to define in solution. In this presentation the use of time-resolved infrared spectroscopy to resolve such photo-induced dynamics in solution and in the crystal state will be described. This talk will examine how the atomic resolution of X-ray crystallography can be combined with ultrafast infrared spectroscopic data to define both the geometry of the reaction site and the rates of individual steps in a reversible photo-induced electron transfer process from a guanine base.

Carrie Wilmot (University of Minnesota, Minneapolis)

MauG catalysis: a tale of ferryl iron, radicals and long distance hopping

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Methylamine dehydrogenase (MADH) is a periplasmic enzyme found in a range of methylotrophic / autotrophic bacteria that enables the organisms to grow on methylamine as a sole source of carbon and energy. Catalytic activity requires the posttranslational modification of two Trp residues in MADH to form the 2-electron redox cofactor tryptophan tryptophylquinone (TTQ), in which two carbonyl oxygens have been added to one of the Trp indole rings, and the two Trp residues crosslinked. Maturation of MADH requires the expression of four accessory genes. One of these is a di-heme enzyme, MauG, which catalyzes the completion of TTQ biosynthesis in a 6-electron oxidation. The key MauG catalytic intermediate is a *bis*-Fe(IV) species comprised of a ferryl heme (Fe(IV)=O) with the second heme in the Fe(IV) oxidation state. The *bis*-Fe(IV) MauG is extremely sensitive to photoreduction in the X-ray beam reducing through diferric (Fe(III)) to the fully reduced diferrous (Fe(II)) MauG. A range of single crystal spectroscopies have been explored to track photoreduction (UV-visible absorbance, X-ray absorption spectroscopy, near-IR and resonance Raman). Completion of TTQ to generate active MADH involves long-range electron transfer and a radical hopping mechanism to effect catalysis over a 40 Å distance. The MauG catalyzed reaction occurs in three discrete 2-electron events in a H₂O₂ or O₂-dependent process. A crystal structure of MauG in complex with its protein substrate, a precursor form of MADH known as preMADH, has been solved. The crystals are catalytically active. The order of the 2-electron chemistry catalyzed by MauG was determined in the crystal and corroborated by mass spectrometry in solution. This talk will give background on studying enzyme reactions within crystals, and detail how we combined

crystallography, spectroscopy and mass spectrometry to determine the order of chemistry in TTQ biosynthesis, and in our efforts to solve the X-ray crystal structure of the photosensitive *bis*-Fe(IV) MauG catalytic intermediate.