Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

CUI THE HAMBURG CENTRE FOR ULTRAFAST IMAGING

CLUSTER OF EXCELLENCE
CUI: ADVANCED IMAGING OF MATTER

The Hamburg Centre for Ultrafast Imaging

The Graduate Days 2019

Hamburg
March 18 – 21

DESY

European XFEL

MAX-PLANCK-GESELLSCHAFT

Contents

Programme

Monday, March 18, 2019

9:30 **Prof. Klemens Hammerer and Dr. Sahand Mahmoodian**
Light-matter quantum interfaces: Optomechanics and chiral quantum optics
(ZOQ, bld. 90, seminar room, ground floor)

Prof. Jens Bredenbeck
2D-IR spectroscopy: Protein dynamics, ultrafast structure determination and steering photochemistry
(CFEL, bld. 99, seminar room I, ground floor)

Dr. Klaas Giesbertz
Density functional theory
(CFEL, bld. 99, seminar room II, ground floor)

10:50 Coffee break (ZOQ, CFEL)

11:10 **Prof. Klemens Hammerer and Dr. Sahand Mahmoodian**
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(CFEL, bld. 99, seminar room II, ground floor)

12:30 Lunch break

14:00 **Dr. Richard Schmidt**
Polaron physics in ultracold atoms and solid-state materials
(ZOQ, bld. 90, seminar room, ground floor)

Prof. Wilfried Wurth
Femtochemistry and surface physics
(CFEL, bld. 99, seminar room I, ground floor)

Dr. Thomas Braun
Cellular imaging and nanoanalytics to study neurodegeneration: From nanomechanical sensors to single cell visual proteomics
(CFEL, bld. 99, seminar room II, ground floor)

Tuesday, March 19, 2019

9:30 **Prof. Klemens Hammerer and Dr. Sahand Mahmoodian**
Light-matter quantum interfaces: Optomechanics and chiral quantum optics
(ZOQ, bld. 90, seminar room, ground floor)

Prof. Jens Bredenbeck
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Dr. Thomas Braun
Cellular imaging and nanoanalytics to study neurodegeneration: From nanomechanical sensors to single cell visual proteomics
(CFEL, bld. 99, seminar room II, ground floor)

15:30 Free time

17:00 Colloquium
Prof. Päivi Törmä
New perspectives on quantum geometry, superconductivity and Bose-Einstein condensation
(CFEL, bld. 99, seminar rooms I-II-III)

18:00 Reception (CFEL, bld. 99, Foyer)

Wednesday, March 20, 2019

9:30 **Prof. Klemens Hammerer and Dr. Sahand Mahmoodian**
Light-matter quantum interfaces: Optomechanics and chiral quantum optics
(ZOQ, bld. 90, seminar room, ground floor)

Prof. Jens Bredenbeck
2D-IR spectroscopy: Protein dynamics, ultrafast structure determination and steering photochemistry
(CFEL, bld. 99, seminar room I, ground floor)

Dr. Klaas Giesbertz
Density functional theory
(CFEL, bld. 99, seminar room II, ground floor)

10:50 Coffee break (ZOQ, CFEL)

11:10 **Prof. Klemens Hammerer and Dr. Sahand Mahmoodian**
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Dr. Klaas Giesbertz
Density functional theory
(CFEL, bld. 99, seminar room II, ground floor)

12:30 Lunch break

14:00 **Dr. Richard Schmidt**
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(ZOQ, bld. 90, seminar room, ground floor)

Prof. Wilfried Wurth
Femtochemistry and surface physics
(CFEL, bld. 99, seminar room I, ground floor)

Dr. Thomas Braun
Cellular imaging and nanoanalytics to study neurodegeneration: From nanomechanical sensors to single cell visual proteomics
(CFEL, bld. 99, seminar room II, ground floor)

15:30 Free time

16:30 Industry event
Dr. Stephan Ritter
Quantum technologies: from basic research to industry
(CFEL, bld. 99, seminar rooms I-II)

17:30 **Reception** (CFEL, bld. 99, Foyer)

Thursday, March 21, 2019

9:30 **Bernd Klein**
Machine learning in Python: A step-by-step hands-on introduction
(Bld. 61, Rechnerraum/CIP Pool, ground floor)

Prof. Gerwald Lichtenberg
Multidimensional data analysis with MATLAB
(Bld. 3, room 3, ground floor)

Dr. Andrew Wold
Scientific presentation skills
(CFEL, bld. 99, seminar room V, 1st floor)

Dr. Sabine Baars
Options for third party funding and how to apply
(CFEL, bld. 99, seminar room 01.060, 1st floor)

10:50 Coffee break (Bld. 3, bld. 61, CFEL)

11:10 **Bernd Klein**
Machine learning in Python: A step-by-step hands-on introduction
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15:20 Coffee break (Bld. 3, bld. 61, CFEL)

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17:00 End of the Graduate Days

Abstracts

Morning long courses (Mon-Wed, 9:30-12:30)

<u>Light-matter quantum interfaces: Optomechanics and chiral quantum optics</u>

Prof. Klemens Hammerer and Dr. Sahand Mahmoodian (Leibniz Universität Hannover, Germany)

In our lecture we will provide an introduction to quantum interfaces between light and matter. We will explain how material degrees of freedom, in particular of cold trapped atoms, quantum dots, and micromechanical oscillators, can be coupled highly efficiently to one-dimensional guided modes of light. Such light-matter interfaces can then be used to interconnect ensembles of atoms and even hybrid setups of atoms and mechanical oscillators when these systems are coupled to propagating light fields in a cascaded fashion. In this way it is possible to engineer the quantum state of distant material degrees of freedom, for example, to cool to quantum mechanical ground states or to generate entangled states, as well as to engineer the quantum state of light transmitted through an ensemble of cascaded atoms.

<u>Prerequisites for attending the lecture:</u>

Interfacing single photons and single quantum dots with photonic nanostructures, Peter Lodahl, Sahand Mahmoodian, and Søren Stobbe, Rev. Mod. Phys. 87, 347 (2015), arXiv:1312.1079

Chiral quantum optics, Peter Lodahl, Sahand Mahmoodian, Søren Stobbe, Arno Rauschenbeutel, Philipp Schneeweiss, Jürgen Volz, Hannes Pichler, and Peter Zoller, Nature 541, 473 (2017), arXiv:1608.00446

Quantum interface between light and atomic ensembles, Klemens Hammerer, Anders S. Sørensen, and Eugene S. Polzik, Rev. Mod. Phys. 82, 1041 (2010), arXiv:0807.3358

Hybrid Mechanical Systems, Philipp Treutlein, Claudiu Genes, Klemens Hammerer, Martino Poggio, and Peter Rabl, in: "Cavity Optomechanics", ed. by M. Aspelmeyer, T. J. Kippenberg, and F. Marquardt (Springer, Berlin 2014) pp. 327-351, arXiv:1210.4151

<u>2D-IR spectroscopy: Protein dynamics, ultrafast structure determination and steering photochemistry</u>

Prof. Jens Bredenbeck (Institute of Biophysics, Goethe Universität Frankfurt, Germany)

We will briefly cover the basics of molecular vibrations and infrared spectroscopy. We will explore the information content of static and time resolved infrared spectra using examples from chemistry and biology. Based on this foundation, ultrafast 2D-IR spectroscopy will be introduced. In contrast to 1D spectroscopy, 2D-IR spectroscopy reveals cross-peaks between bands of the IR absorption spectrum. We will discuss different mechanisms of how such cross-peaks are generated, such as chemical exchange, spectral diffusion, anharmonic coupling and vibrational energy transfer and how they can be exploited to investigate molecular structure and dynamics on a time scale of ~100 fs and longer.

Augmenting IR pulse sequences with near-IR, Vis or UV pulses creates novel spectroscopies, such as transient 2D-IR, triggered exchange 2D-IR, surface specific 2D-IR or VIPER 2D-IR. We will discuss the information content and application range of these mixed IR / non-IR multidimensional spectroscopies, using examples from protein biophysics, photochemistry, surface chemistry and others.

If time permits, technical aspects and different approaches of collecting 2D-IR spectra will be explained, comparing their advantages and disadvantages.

<u>References:</u>

From ultrafast structure determination to steering reactions: mixed IR/non-IR multidimensional vibrational spectroscopies, Luuk J. G. W. van Wilderen, Jens Bredenbeck, Angew. Chem. Int. Ed. 54, 11624-11640 (2015).

Concepts and Methods of 2D Infrared Spectroscopy, Peter Hamm and Martin Zanni, Cambridge University Press (2011).

Density functional theory

Dr. Klaas Giesbertz (Vrije Universiteit Amsterdam, The Netherlands)

In this course I will explain the theoretical aspects of Density Functional Theory (DFT). The foundations of DFT will be built up from general considerations, to help you understand how DFT fits in a larger picture of methods aiming to deal with the quantum many-particle problem. We will go through the derivation of the Kohn-Sham equations and discuss their function and importance for the performance of practical DFT. I will also explain the philosophy used in the construction of basic approximations to the remaining exchange-correlation functional (LDA, GGA, hybrid) and point out important features of their performance. If time permits, I will also discuss the interpretation of the Kohn-Sham orbitals and orbital energies.

Prerequisites for attending the lecture: Basic Quantum Mechanics, basic linear algebra and Lagrange multipliers (Wikipedia / lectures notes Appendix B)

Afternoon short courses (Mon-Wed, 14:00-15:30)

Polaron physics in ultracold atoms and solid-state materials

Dr. Richard Schmidt (Max Planck Institute of Quantum Optics, Garching, Germany)

When an impurity is immersed into an environment, it changes its properties due to its interactions with the surrounding medium. Indeed, the impurity becomes dressed by excitations in the environment and may form a quasiparticle called polaron. Polarons feature altered properties such as an effective mass and a modified response to external perturbations.

In this lecture, I will introduce the concept of polaron formation and present recent experimental and theoretical progress on studying a variety of polaronic phenomena. After giving an overview over various types of polaronic states found in solid state systems, physical chemistry, and ultracold atomic gases, I will explain how polarons can be theoretically described by means of simple variational wave functions. To this end, I will focus on the problem of a mobile quantum impurity interacting with a Fermi gas which forms a so-called Fermi polarons. After discussing the observation of Fermi polarons in experiments with cold atomic systems, we will turn to two-dimensional materials where polaron physics has recently become a focal point of research. First, we will briefly introduce two-dimensional semiconductors where the interaction between excitons and electrons leads to polaron formation. After reviewing excitons, we will then apply Fermi polaron theory to demonstrate how the optical properties of atomically thin semiconductor heterostructures can be manipulated by exploiting polaronic effects.

In the last part of this lecture we will turn to the famous Anderson orthogonality catastrophe which deals with the breakdown of the polaron description. The Anderson orthogonality catastrophe takes place in systems where the mass of the impurity approaches infinity, and the generation of an infinite number of low-energy excitations may destroy the quasiparticle. We will briefly discuss how this situation can be described theoretically, and we then relate our findings to current frontiers in research where the formation and destruction of polarons is currently explored.

Prerequisites for attending the lecture: Quantum Mechanics

Femtochemistry and surface physics

Prof. Wilfried Wurth, Center for Free-Electron Laser Science, Universität Hamburg and DESY Photon Science

The study of chemical reactions at surfaces is one of the central research areas in surface science. It is motivated by the importance of heterogenous catalysis for many applications relevant to society. With the availability of X-ray free-electron lasers many of the techniques used to investigate the kinetics of surface chemical reactions can now be used to probe the real-time dynamics of these reactions on sub-picosecond timescales.
In the first lecture an overview on standard concepts in surface physics and the investigation of surface chemical reactions will be given. The second lecture will cover studies of the real-time dynamics of surface chemical reactions performed with short

pulse laser sources in the lab. Finally, recent results obtained at X-ray free-electron lasers will be discussed and perspectives for future research will be presented.

Cellular imaging and nanoanalytics to study neurodegeneration: From nanomechanical sensors to single cell visual proteomics

Dr. Thomas Braun (Center for Cellular Imaging and Nanoanalytics, Universität Basel, Switzerland)

The three lectures present new methods for the biomedical imaging and nanoanalysis of cellular systems and their application to the study of neurodegenerative diseases.

The first lecture will provide a general overview of neurodegenerative diseases, the state of current research, and the limitations of present analytical methods. Neurodegenerative disorders such as Parkinson's disease (PD) and Alzheimer's disease (AD) mainly affect the elderly, and due to demographic shifts, they are afflicting an increasing number of people. Unusual intra- and extracellular aggregates are closely associated with PD and AD. These "plaques" are related to disease-specific misfolded proteins. A stereotypical spreading of these plaques throughout the brain is typical in these disorders. The model of the "prion-like spreading" of aggregates containing misfolded proteins provides an elegant explanation for this phenomenon. However, the detailed mechanism for this spreading is unknown, and different pathways have been suggested. The lecture will provide an overview of neurodegenerative diseases and ongoing research.

The second lecture will provide an overview of nanomechanical sensors and their application in biomedical research. Since the invention of the atomic force microscope by Binnig, Quate, and Gerber in 1986, many different applications have been invented. The lecture will provide a historical overview of the various modes of the atomic force microscope and its siblings, nanomechanical sensors. Whenever possible, the focus will be on biomedical applications for the study of neurodegenerative diseases.

The third lecture will provide an overview of microfluidic sample preparation methods for electron microscopy and the new opportunities arising thereof. During recent years, direct electron detection cameras for electron microscopes (EM) introduced a rapid and lasting advance to structural biology, and are now regarded as a standard method for the structural analysis of protein complexes to atomic resolution. However, protein isolation techniques and sample preparation methods for cryo-EM remain a bottleneck. For a high-resolution analysis of proteins by the cryogenic EM (cryo-EM) single-particle approach, only 10’000 to a few million individual protein particles must be imaged. Therefore, microfluidic techniques can provide enough protein complexes for the structural investigation by cryo-EM and the single-particle approach. We developed microfluidic methods for the sample preparation for electron microscopy, consuming only a few nanoliters of the specimen in total. The lecture will provide an overview over microfluidics and EM sample preparation in general and will highlight new experimental approaches for the single-cell analysis not possible before.

Prerequisites for attending the lecture: All three presentations will discuss basic concepts and no prior knowledge is needed.

Practical and soft-skills workshops (Thu, 9:30-17:00)

Machine learning in Python: A step-by-step hands-on introduction

Dipl.-Inform. Bernd Klein (Bodenseo, Singen, Germany)

1. Getting and Familiarizing with Python and its ML Modules:
   scipy
   numpy
   matplotlib
   pandas
   sklearn
   PyCharm, Spyder and Jupyter-Notebook
2. Examining the Data Sets:
   The "Hello-World" of Machine Learning: Iris Dataset
3. Visualization of the Data
4. Classifying the Data by using
   a) nearest-Neighbour Classifier
   b) Neural Networks

Prerequisites for attending the lecture: Intermediate Programming Skills in some programming language, e.g. C, C++, Java.

Multidimensional data analysis with MATLAB
Prof. Gerwald Lichtenberg (Hochschule für Angewandte Wissenschaften, Hamburg, Germany)

Scientific computation tools support 2D data as a standard because data analysis and visualisation algorithms often are defined for matrices. But in a lot of research fields and applications, data is naturally structured along more than two axes and 3D, 4D, or in general multidimensional arrays are appropriate. Elements of these are stored and accessed by three or more indices, which reflects neighbourhood relations that might be lost in matrix representation.

Moreover, tensor decomposition methods are available for multidimensional arrays which are intensively studied in many disciplines: independent component analysis, blind source separation, signal processing, data mining, system modelling, audio and image processing, biomedical applications, bio-informatics, and many more. In contrast to machine learning algorithms, tensor decompositions can lead to interpretable factors as results. These methods have mathematical roots in multilinear algebra, algebraic geometry and optimization.

The workshop will introduce modern methods and tools for multidimensional data analysis as *Tensorlab* and the *Tensor Toolbox* based on MATLAB. Examples will be given and participants are encouraged to bring own data samples.

Prerequisites for attending the lecture:
Linear algebra basics
MATLAB basics

Scientific presentation skills
Dr. Andrew Wold (Project Manager at GRASP, Linköping University, Sweden)

The ability to present scientific research is a skill that some have, but others need to hone. This course will provide participants with practical knowledge to better structure and deliver their scientific research. Furthermore, this course will work on presentation skills that will prepare students to present not only research content, but also themselves. As most students will look to further their academic careers, it is important to optimally present yourself for future interviews. This course will help participant's present confidently and effectively.

Methods: Group and individual exercises, improvisation methods, presentation theory, trainer feedback

Options for third party funding and how to apply
Dr. Sabine Baars (Universität Hamburg, Germany)

Colloquium (Tue, 17:00)

New perspectives on quantum geometry, superconductivity and Bose-Einstein condensation
Prof. Päivi Törmä (Department of Applied Physics, Aalto University, Finland)

Superconductivity, superfluidity and Bose-Einstein condensation (BEC) are many-body phenomena where quantum statistics are crucial and the effect of interactions may be intriguing. Superconductors are already widely applied, but theoretical understanding of superconductivity and condensation in several real world systems is still a challenge, and superconductivity at room temperature remains a grand goal. We have recently discovered that superconductivity (superfluidity) has a connection to quantum geometry [1-3]. Namely, the superfluid weight in a multiband system has a previously unnoticed component, which we call the geometric contribution. It is proportional to the quantum metric of the band. Quantum metric is connected to the Berry curvature, and this allows to relate superconductivity with the topological properties of the band. Using this theory, we have shown that superconductivity is possible also in a flat band where individual electrons would not move. We show that, in a flat band, the salient features of superconductivity are actually given already by the two-body physics [3]. These results may be essential in explaining for instance the recent observation of superconductivity in bilayer graphene, and may eventually help realize superconductors at elevated temperatures.

Bose-Einstein condensation has been realized for various particles or quasi-particles, such as atoms, molecules, photons, magnons and semiconductor exciton polaritons. We have recently experimentally realized a new type of condensate: a BEC of hybrids of surface plasmons and light in a nanoparticle array [4]. The condensate forms at room temperature and shows ultrafast dynamics. We utilized a special measurement technique, based on formation of the condensate under propagation of the plasmonic excitations, to monitor the sub-picosecond thermalization dynamics of the system. This new platform is ideal for studies of differences and connections between BEC and lasing [5], and eventually also studies of topological phenomena due to the easy tunability of the array geometry and the system symmetries [6].

[1] S. Peotta, P. Törmä, Nature Communications **6**, 8944 (2015)
[2] A. Julku, S. Peotta, T.I. Vanhala, D.-H. Kim, P. Törmä, Physical Review Letters **117**, 045303 (2016)
[3] P. Törmä, L. Liang, S. Peotta, Physical Review B Rapid Communication,
[4] T.K. Hakala, A.J. Moilanen, A.I. Väkeväinen, R. Guo, J.-P. Martikainen, K.S.
Daskalakis, H.T. Rekola, A. Julku, P. Törmä, Nature Physics **14**, 739 (2018)
[5] T.K. Hakala, H.T. Rekola, A.I. Väkeväinen, J.-P. Martikainen, M. Necada, A.J. Moilanen, and P. Törmä, Nature Communications **8**, 13687 (2017)
[6] R. Guo, M. Necada, T.K. Hakala, A.I. Väkeväinen, P. Törmä, Physical Review Letters **122**, 013901 (2019)

Industry event talk (Wed, 16:30)

<u>Quantum technologies: from basic research to industry</u>

Dr. Stephan Ritter (TOPTICA Photonics AG, Gräfelfing / Munich, Germany)

Quantum effects not only provide deeper insights into fundamental physics, but can also be exploited to advance a broad range of technologies. They promise higher precision in sensing and metrology, a new computing paradigm, fundamental advantages in secure communication and much more. Inventing these protocols and applications is one of the great tasks for theorists, while the experimental challenge is to gain full control over the employed quantum systems. Their reliable production and manipulation at the quantum level often requires either the most advanced classical technologies or even a new generation of devices. We are currently witnessing an exciting transition of quantum technologies from academic labs into industry, as can for example be seen from the quickly growing number of quantum technology startups.

TOPTICA Photonics is deeply rooted in the quantum technology community from which it emerged more than 20 years ago. Since then, TOPTICA develops and manufactures high-end laser systems for scientific applications and industrial applications. In my talk, I will present some of the opportunities and challenges TOPTICA faces by providing enabling technologies for the rapidly developing market of quantum technologies and give examples of TOPTICA's direct involvement in this new field, e.g. the development of an optical atomic clock.

Last but not least, my own career path serves as a good example for the entanglement between academic research and industry. I will sketch how my curiosity for quantum effects and enthusiasm for technology took me from developing a laser as a student at Universität Hamburg to research on ultracold quantum gases at ETH Zurich, to building quantum networks at MPQ in Munich, and to finally become TOPTICA's Application Specialist for Quantum Technologies.

<u>Prerequisites for attending the lecture:</u> none

Practical information

Organisation

Antonio Negretti, Anja Cordes, and Jutta Voigtmann

Location

Campus Bahrenfeld
Notkestraße 85 (main entrance)/Luruper Chaussee 149 (side entrance)

- Center for Free-Electron Laser Science (CFEL), building 99
- Center for Optical Quantum Technologies (ZOQ), building 90
- Building 03
- Building 61

Contact

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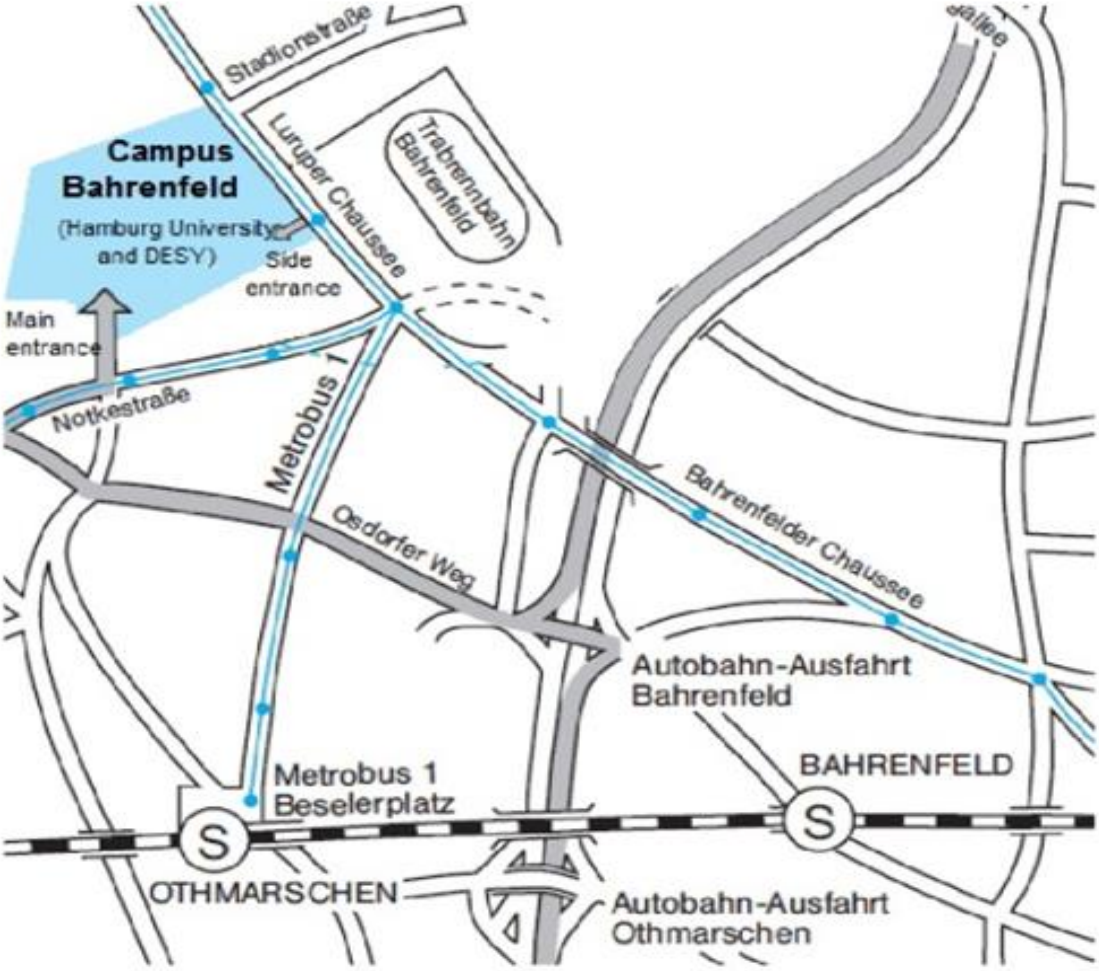
E-mail: anegrett@physnet.uni-hamburg.de

Directions



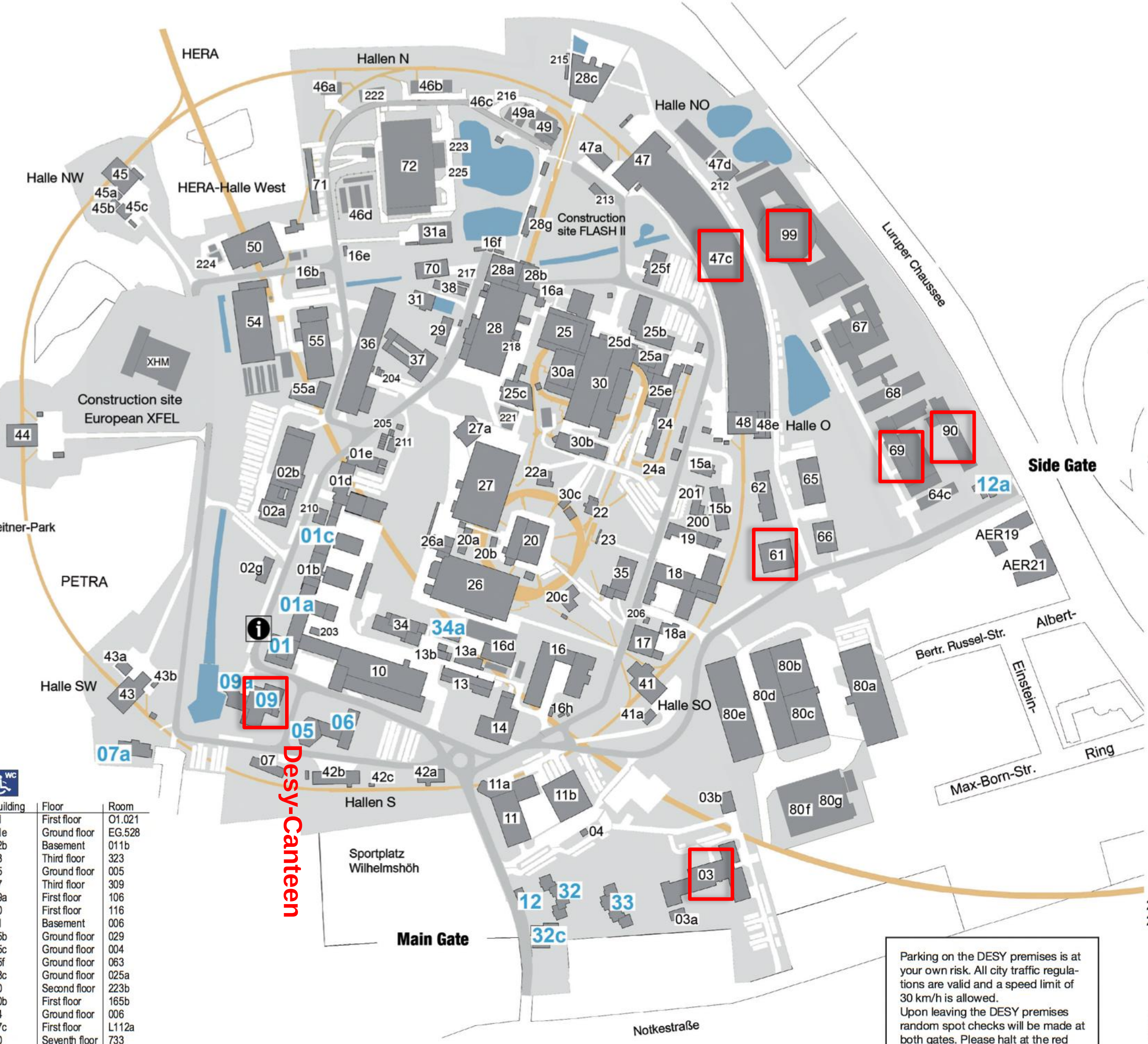
By train: to Hamburg-Altona station, then continue by taxi (travelling time about 15 minutes) or take a bus (see below).

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 about 20 minutes.

From train station “S-Bahn Othmarschen”, take bus line 1 (direction “Rissen/Blankenese“) directly to the main entrance of the campus (bus stop “Zum Hünengrab/DESY“), travelling time about 25 minutes.

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

Laboratory 1	01-01e
Directorate	**01**
Press and public relations	**01**
Company medical officer	**01a**
Library	**01d**
Laboratory 2a, Theory	02a
Computer Centre, UCO	02b
Laboratory	02g
Laboratory 3	03
Caretaker	03a
Storage building	03b
Gas station	04
Auditorium, entrance building 6	05
Administration building, **Guest services**	**06**
Administration building	07
Guest house 8	**07a**
Cafeteria, Bank	**09**
Bistro	**09a**
Workshop	10
Purchasing department	11
Central warehouse	11a
Cable hall	11b
Gate lodge Notkestraße (main gate)	**12**
Gate lodge Luruper Chaussee (side gate)	**12a**
Liquifying plant	13
Gas cylinder building	13a
Helium container building	13b
Vacuum laboratory	14
Office building	15a, b
Power station	16
10 kV main station	16a, b
Cooling plant DESY II	16d
Filter network switchyard	16e
Emergency power switch facility	16f
Storage building	16h
Heating plant	17
Maintenance building	18, 18a
Carpenters' building	19
Synchrotron building	20
Filtering hall	20a
10 kV substation 5a	20b
Power house DESY	20c
Vacuum engineering	22
Laboratory of the Universities of Hamburg and Lübeck	22a
LINAC I	23
LINAC II	24
PIA	24a
HASYLAB laboratory	25
EMBL	25a
HASYLAB laboratory 1, MPG	25b
HASYLAB X-ray wiggler hall, HZG / GFZ	25c
HASYLAB laboratory 4	25d
HASYLAB laboratory 5	25e
HASYLAB laboratory 2	25f
LINAC III / experimental hall I	26
FLA laboratory	26a
Experimental hall II	27
Testing area	27a
TTF / experimental hall III	28
Cryogenic hall	28a
FLASH tunnel	28b
FLASH experimental hall	28c
FLASH laser hut	28g
Iron removal plant	29



WC

Building	Floor	Room
01	First floor	01.021
01e	Ground floor	EG.528
02b	Basement	011b
03	Third floor	323
05	Ground floor	005
07	Third floor	309
09a	First floor	106
10	First floor	116
11	Basement	006
25b	Ground floor	029
25c	Ground floor	004
25f	Ground floor	063
28c	Ground floor	025a
30	Second floor	223b
30b	First floor	165b
34	Ground floor	006
47c	First floor	L112a
50	Seventh floor	733
55	Ground floor	007
72	Ground floor	EG.005
72	Second floor	02,203

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Upon leaving the DESY premises random spot checks will be made at both gates. Please halt at the red traffic signal or the horn signal for inspection.

30	Storage ring DORIS / experimental hall IV
30a	DORIS supplying hall
30b	Accelerator operation building
30c	Power station
31a	Accelerator components building
32	**Guest house 2**
32c	**Kindergarten**
33	**Guest house 3**
34	Training area
34a	**physik.begreifen@desy.de**
35	Safety group / Communication engineering
36	Preparation hall, experimental hall V
37	Assembly hall
38	Storage building
41, 41a	PETRA halls SO
42, a-c	PETRA halls S
43a, b	PETRA halls SW
44	PETRA hall W
45, a-c	PETRA halls NW
46a-c	PETRA halls N
46d	Power station, cooling plan
47, a	PETRA halls NO
47c	PETRA III experimental hall
47d	PETRA III cooling plant
48, e	PETRA halls O / EMBL
49, 49a	Office building
50	HERA hall west
54	Refrigeration technology hall
55	Magnet measurement hall
55a	Proton vacuum building
61-69	University Hamburg
61	Auditorium
62	Institute of experimental physics
64c	Preparation building
65	Workshop
66	Theory
67	Institute of experimental physics
68	Institute of experimental physics
69	Institute of laser physics
70	Modul test hall
71	XTL mock up
72	AMTF hall
80a-g	Storage buildings
90	Zentrum für Optische Quantentechnologie (ZOQ)
99	CFEL
200	Office container MPG
201	Office container MPG
202-207	Container
210-218	Container

Off-site buildings:

51	HERA hall north
52	HERA hall east
53	HERA hall south
AER19	European XFEL
AER21	Project management agency PT-DESY

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