

The Hamburg Centre for Ultrafast Imaging The Graduate Days 2017

Hamburg March 13 – 16











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Programme

Monday, March 13, 2017

8:30 Registration (CFEL, Bld. 99, Foyer)

9:30 Dr. Davide Rossini Many-body physics in open quantum systems (ZOQ, Bld. 90, Seminar room, ground floor)

> **Dr. Hans Behringer** Introduction to molecular dynamics simulations (CFEL, Bld. 99, Seminar room I-II, ground floor)

Prof. Gerhard Nägele

Structure and dynamics of colloidal soft matter (ILP, Bld. 69, Seminar room, ground floor)

10:50 Coffee Break (CFEL, ILP, ZOQ)

11:10 Dr. Davide Rossini

Many-body physics in open quantum systems (ZOQ, Bld. 90, Seminar room, ground floor)

Dr. Hans Behringer

Introduction to molecular dynamics simulations (CFEL, Bld. 99, Seminar room I-II, ground floor)

Prof. Gerhard Nägele

Structure and dynamics of colloidal soft matter (ILP, Bld. 69, Seminar room, ground floor)

12:30 Lunch (DESY-Canteen, Bld. 09)

14:00 Dr. Christian Ott

Attosecond flashes of light: Illuminating electronic quantum dynamics (ZOQ, Bld. 90, Seminar room, ground floor)

Prof. Steve Meech

Photodynamics in biomolecular systems (CFEL, Bld. 99, Seminar room I-II, ground floor)

Prof. Stefan Eisebitt

Ultrafast x-ray scattering and holography (ILP, Bld. 69, Seminar room, ground floor)

15:30 Free time

Tuesday, March 14, 2017

9:30 Dr. Davide Rossini Many-body physics in open quantum systems (ZOQ, Bld. 90, Seminar room, ground floor)

> **Dr. Hans Behringer** Introduction to molecular dynamics simulations (CFEL, Bld. 99, Seminar room I-II, ground floor)

> **Prof. Gerhard Nägele** Structure and dynamics of colloidal soft matter (ILP, Bld. 69, Seminar room, ground floor)

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(CFEL, Bld. 99, Seminar room I-II, ground floor)

Prof. Stefan Eisebitt

Ultrafast x-ray scattering and holography (ILP, Bld. 69, Seminar room, ground floor)

- 15:40 Lab tour #1
- 16:20 Lab tour #2
- 17:00 Colloquium Prof. Elspeth Garman 104 years of chrystallography: what has it taught us and where will it lead us? (CFEL, Bld. 99, Seminar rooms I-II-III)
- 18:00 Barbeque (CFEL, Bld. 99, Foyer)

Wednesday, March 15, 2017

9:30 Dr. Davide Rossini Many-body physics in open quantum systems (ZOQ, Bld. 90, Seminar room, ground floor)

Dr. Hans Behringer

Introduction to molecular dynamics simulations (CFEL, Bld. 99, Seminar room I-II, ground floor)

Prof. Gerhard Nägele

Structure and dynamics of colloidal soft matter (ILP, Bld. 69, Seminar room, ground floor)

10:50 Coffee Break (CFEL, ILP, ZOQ)

11:10 Dr. Davide Rossini

Many-body physics in open quantum systems (ZOQ, Bld. 90, Seminar room, ground floor)

Dr. Hans Behringer

Introduction to molecular dynamics simulations (CFEL, Bld. 99, Seminar room I-II, ground floor)

Prof. Gerhard Nägele Structure and dynamics of colloidal soft matter (ILP, Bld. 69, Seminar room, ground floor)

12:30 Lunch (DESY-Canteen, Bld. 09)

14:00 Dr. Christian Ott

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Ultrafast x-ray scattering and holography (ILP, Bld. 69, Seminar room, ground floor)

- 15:30 Free time
- 16:30 Industry event

Dr. Alexander van Staa and Dr. Johanna Busch NXP semiconductors – Secure connections for a smarter World (CFEL, Bld. 99, Seminar rooms I-II-III)

17:30 Reception (CFEL, Bld. 99, Foyer)

Thursday, March 16, 2017

9:30 Bernd Klein

Introduction into Phyton for scientists (Physics department, Jungiusstr. 9, 20355 Hamburg, Pool room 3 – No. 302, 3rd floor)

Bodo P. Krause-Kyora

Matlab: Introduction and real world use-case for measurements and simulation (Physics department, Jungiusstr. 9, 20355 Hamburg, Pool room 1 – No. 306, 3rd floor)

Rob Thompson

Communication – Negotiate – Resolve In cooperation with the PIER Helmholtz Graduate School (Bahrenfeld Campus, CFEL, Bld. 99, room 02.104, 2nd floor)

Dr. Peter Schröder

Project management throughout the doctorate: From conception to implementation everything under control (Bahrenfeld Campus, CFEL, Bld. 99, Seminar room IV, 1st floor)

Dr. Simon Golin

Project management in academia: From conception to implementation everything under control

(Bahrenfeld Campus, CFEL, Bld. 99, Seminar room V, 1st floor)

10:50 Coffee Break (CFEL, Physics Dep.)

11:10 Bernd Klein

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12:30 Lunch (DESY-Canteen; Bld. 09 resp. Bucerius Law School Canteen, Jungiusstraße 6)

14:00 Bernd Klein

Introduction into Phyton for scientists (Physics department, Jungiusstr. 9, 20355 Hamburg, Pool room 3 – No. 302, 3rd floor)

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15:20 Coffee Break (CFEL, Physics Dep.)

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17:00 End of the Graduate Days of CUI

Abstracts

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

<u>Many-body physics in open quantum systems</u>: Dr. Davide Rossini (Scuola Normale Superiore di Pisa, Pisa, Italy)

The recent development of quantum technologies has drastically enhanced our capability to control quantum coherence at the level of the single particle in a variety of physical systems, ranging from atomic and molecular optics, to trapped ions, semiconducting nanodevices, and cavity/circuit quantum electrodynamics (QED). In several cases, it is even possible to control the action of the coupling to an external environment, such as for certain quantum optical systems and for coupled QED cavities. The system can be thus driven, with a good accuracy, into specific quantum states.

As a consequence to these advancements, nowadays the quest for a careful theoretical modeling and study of quantum many-body physics in a driven-dissipative context is crucial, and goes well beyond the simple understanding of the breakdown of quantum coherence. Moreover, one cannot even prescind from a careful treatment of interactions beyond the perturbative limit, since dramatic many-body effects due to strong correlations can be envisaged even in the open scenario.

These lectures will be introduced by an overview of the available experimental platforms where the many-body physics of open quantum systems can be readily accessed and tested. Due to the formidable difficulty in approaching their description, unfortunately most of our theoretical understanding for these systems is limited to the mean-field level, where interactions are treated crudely. I will present the most recent numerical approaches that are able to shed light on the many-body driven-dissipative realm beyond that limit. Specifically, I will provide a pedagogical introduction to a variety of methods including quantum trajectories, matrix product operators, cluster mean-field approaches, and linked cluster expansions. I will then show how one can envisage a combination of some of them in order to extend their capabilities in treating larger systems and higher dimensionalities.

In the second part of my lectures, I will enter the details of some interesting results that have been recently achieved using the above mentioned

methods. Emphasis will be put on the significant differences that may emerge with respect to the mean-field treatment, after a thorough treatment of the role of interactions. As expected, discrepancies generally become more pronounced in a reduced dimensionality, but can be anyway of fundamental importance even in other subtler contexts, due to the fact that short-range correlations and fluctuations may have a dramatic influence.

The range of outcomes that I will present includes the characterization of exotic quantum phases that can be stabilized in non-equilibrium steady states under driven-dissipative conditions, the quantum transport properties in a non-perturbative interacting regime for the open scenario, and some prominent features of the steady-state many-body phase diagram.

Introduction to molecular dynamics simulations: Dr. Hans Behringer (The Hamburg Centre for Ultrafast Imaging and Universität Hamburg, Hamburg, Germany)

Complex systems with their many degrees of freedom on different length and time scales exhibit fascinating characteristics and properties. Although their description can in principle be formulated in terms of a quantitative theory on the microscopic level, mathematical solutions for particluar systems are hardly feasible. Theoretical investigations into the underlying principles that govern the systems are therefore strongly relying on approximations, however, often systems are to complicated and defy a systematic treatment. An alternative route to look into such problems is provided by computational physics where simulations on a computer are used to reproduce and eventually understand the behaviour of systems.

This lecture course is directed at students with no background in computational physics and gives an introduction to the basics of classical molecular dynamics simulations. The lecture develops and discusses why and how this method works and demonstrates its practical application for simple physical problems. After having established the key ingredients of molecular dynamics simulations the lecture concentrates on a particular example from current research, namely the modelling and simulation of protein dynamics. The lecture will finally give an outlook to more advanced methods.

<u>Structure and dynamics of colloidal soft matter</u>: Prof. Gerhard Nägele (Institute of Complex Systems, ICS-3 and Forschungszentrum Jülich GmbH, Jülich, Germany) Mesoscale particles dispersed in a viscous fluid are found in numerous technological processes and products including paints, pharmaceuticals and food products, and in biological systems such as cells. The particles size spans a broad range, from micron-sized synthetic colloidal particles down to nano-sized proteins and even smaller electrolyte The ions. equilibrium microstructure. thermodynamics and phase behavior of colloidal systems is determined by direct particle interaction including van der Waals attraction and steric repulsion, and screened Coulomb repulsion in case charged particles. Additionally of to direct interactions, the colloid dynamics is strongly influenced by Brownian motion, and by the longinteraction range hydrodynamic particle (HI) transmitted quasi-instantaneously by the solvent flow. The HI gives rise to a plethora of phenomena that are often unexpected. It changes the diffusion and rheological properties of concentrated dispersions, and it affects the kinetic pathways and resulting phase diagram in non-equilibrium phase transitions.

In this lecture series, I give an overview over the statistical physics and low-Reynolds number hydrodynamics of globular colloidal particles undergoing correlated Brownian motion in a Newtonian fluid. Theoretical methods are described allowing for the calculation of microstructural, diffusion, rheological and electro-kinetic properties characterizing a colloidal system. Applications of these methods to experimental systems are discussed including suspensions of microgels and charge-stabilized particles, and protein solutions. The performance of the methods is illustrated by the comparison with computer simulation results. After an introduction where examples of colloidal dispersions are presented, the following topics are addressed:

Static Properties

The salient concept of effective particle interactions is illustrated for charge-stabilized particles where the microionic degrees of freedom are integrated out, giving rise to renormalized particle charges and electrostatic screening parameters. The subtle question of how effective interactions are related to thermodynamic properties is discussed using the example of the osmotic pressure. Effective pair potentials are used as input to self-consistent Ornstein-Zernike methods for calculating radial distribution functions and static structure factors measured, respectively, in video microscopy and in laser light, x-ray and small-angle neutron scattering experiments. Recent theoretical, experimental and computer simulation results for these functions are

presented for protein solutions with competing short-range attraction and long-range repulsion (SALR systems) where dynamic clustering is observed, and for non-ionic microgels having shortrange soft interactions.

Colloidal Hydrodynamics

I discuss here the friction-dominated, guasi-inertiafree related motion of mesoscale particles and dispersing fluid under low-Reynolds-number conditions. Characteristic features of this peculiar dynamics are described (e.g., kinematic reversibility and instantaneity), and highlighted using illustrative examples and movie clips. The concept of hydrodynamic mobility is introduced, and used to describe theoretically the HI of particles with a confining wall for different hydrodynamic boundary conditions. Moreover, the HI of particles settling in the bulk fluid region is analyzed, and for this purpose an astonishing example of many-particles sedimentation is shown.

• Dynamics of colloidal systems

The configurational evolution of correlated Brownian particles under the influence of direct and hydrodynamic interactions is governed by a manyparticles diffusion equation termed generalized Smoluchowski equation. This equation constitutes the base for the calculation of dispersion-averaged transport properties such as collective and selfdiffusion coefficients and viscosities, and dynamic scattering functions characterizing the suspension as a whole. I shall focus on easy-to-apply analytic methods of calculating transport properties that require the radial distribution function and hydrodynamic mobilities as input and are derived using linear response theory. Recent applications of these methods to suspensions of solvent-permeable microgels and SALR systems (low-salinity lysozyme solutions) are presented, and compared with experimental and computer simulation results. Finally, electro-kinetic effects arising from the noninstantaneous response of the microion clouds surrounding charged colloidal particle are explored, for the examples of colloidal electrophoresis and self-diffusion.

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

Attosecond flashes of light: Illuminating electronic quantum dynamics: Dr. Christian Ott (Max Planck Institute for Nuclear Physics, Heidelberg, Germany) Attosecond technology has been pushing the frontier of time-resolved experiments in the past decades. The bandwidth of such pulses normally covers the extreme ultraviolet part of the electromagnetic spectrum, thus directly accessing bound electronic quantum states and their dynamics via the superposition principle, but research is now also pushing with increased attention towards the xray domain, to access isolated core-level dynamics of atoms, molecules and solids. The pulses typically exist either in precisely timed (with respect to the infrared or optical driving field) trains, or even in an isolated form by using appropriate temporal gating techniques. This lecture series will give an introduction to the field of attosecond physics, and covers both the basic concepts as well as applications to the measurement of multi-electron dynamics.

The first lecture will be dedicated to discuss fundamental concepts of ultrashort laser pulses. Special emphasis is put on the time-frequency correspondence by means of the Fourier transform. Topics such as nonlinear pulse propagation, selfphase modulation and pulse compression, as well as characterization techniques for ultrashort laser pulses will be covered.

In the second part of the lecture series we will discuss several aspects of the generation mechanism of attosecond pulses, i.e., from a spectral perspective, the concept of high-order harmonic generation. This also includes an overview of gating techniques and macroscopic phase matching effects with emphasis to explain the necessary ingredients for the generation of such pulses in the lab. Also their characterization via interferometric cross-correlation methods and temporal gating will be introduced, leading into the discussion of selected experiments that demonstrate electron dynamics on the attosecond timescale.

In the final part of the lecture, special emphasis will be put on very recent developments of attosecond transient absorption spectroscopy. This will cover the concept of the optical dipole response of a quantum system and its manipulation by means of strong electric fields. With emphasis on own research, this topic covers the formation and control of spectroscopic line shapes, and how to relate their appearance to multi-electron dynamics of the investigated system. This includes aspects of the intrinsic interaction of different electron quantum configurations and Fano interference, and how to control these effects experimentally on ultrafast timescales.

<u>Photodynamics in biomolecular systems</u>: Prof. Steve Meech (University of East Anglia, Norwich, United Kingdom)

Understanding dynamics in biological systems is a vast subject. What optical spectroscopists can bring to the party are techniques, which can be applied to complex media and are able to record data that was not previously accessible. In this series of three talks I plan to introduce three experiments, which have in common their reliance on ultrafast laser pulses and their applicability to probing dynamics in biology (mainly in proteins and peptides). The focus will be on methods, which are (or have been) used in my own group, but I will aim to compare and contrast those with other approaches. I will not (could not) attempt to cover the whole field of protein dynamics, and in particular I will hardly touch on NMR or the key role of theory and simulation.

The first lecture will describe the ultrafast optical Kerr effect (OKE) as a probe of structure and dynamics in liquids. OKE is a nonresonant method and among the simplest of the third order nonlinear optical experiments, yet provides an excellent signal-to-noise view of liquid dynamics – a neat illustration of the power of optical heterodyne detection. The OKE will be compared with THz transmission spectroscopy, transient IR, 2D infrared (IR) and dielectric relaxation in the context of a discussion of the dynamics of waters of solvation surrounding peptides and proteins.

The second lecture will focus on time resolved fluorescence. Fluorescence is probably the most widely used spectroscopic tool in biology, largely because it is a background free signal detectable down to the single molecule level. However it can be time resolved, rather easily for picosecond resolution and – with a little more difficulty – on the tens of femtosecond timescale. The methods will be described and illustrated with an application to reactive dynamics in the green fluorescent protein and solvation dynamics as a probe of reactive sites in proteins.

The final lecture will focus on transient vibrational spectroscopies, especially transient IR and femtosecond stimulated Raman spectroscopy (FSRS). These methods will be described and illustrated with applications to fluorescent and

photoactive proteins such as dronpa and the LOV domains.

<u>Ultrafast x-ray scattering and holography</u>: Prof. Stefan Eisebitt (Technische Universität Berlin, Berlin, Germany)

In many areas of physics, the temporal response of a system and its nanoscale structure are coupled. Excitations can drive solids into transient phases, altering the material properties on short timescales and making unusual properties transiently available. For example, optical excitation can turn antiferromagnets into ferromagnets - for a few picoseconds. In complex materials, different phases such as insulating and metallic regions can coexist already in the ground state, with the details of this coexistence (spatially as well as temporally after exciation) defining macroscopic properties. It is thus often helpful to be able to combine spatially and temporally resolved information on the nanometer lengthscale and pico- to femtosecond temporal scale.

In this lecture, I will introduce basic concepts of time resolved (resonant) scattering and holographic imaging using x-rays and extreme UV radiation. Furthermore, the combination of such techniques with spectroscopic information is discussed. After introducing the concepts of x-ray scattering as well as the sources of femtosecond x-ray pulses in the lab and at large scale facilities, I will focus on time resolved x-ray holography. You will see how not only amplitude and phase of an object, but also the appearance of an object at different times or at different x-ray energies can be encoded in a hologram. And if you have recorded a x-ray hologram, do you always have 3D information on your object? The lecture will transport the general concepts in this field with examples from current research, with a variety of examples focusing on ultrafast magnetic phenomena.

Colloquium (Tue, 17:00)

<u>104 years of crystallography: what has it taught</u> <u>us and where will it lead us?</u>: Prof. Elspeth Garman (University of Oxford, Oxford, United Kingdom)

What has the art of the chocolatier got to do with drug discovery, proteins and DNA? The linking

theme is crystals, which allow us to determine the three-dimensional shapes of all sizes of molecules, ranging from the tiny chocolate moiety to the much larger proteins that allow our bodies to function through to the DNA that carries our genetic information. Crystallography was born in 1913 with the determination of the 3-D structure of sodium chloride (salt) by the Bragg father and son team. It has flowered to elucidate many disciplines since then, with applications in engineering, physics, chemistry, earth sciences and biology. Using crystallography, we can unravel the shapes of biomolecules in our bodies that are targets for drugs against disease, and thus identify new treatments. I will focus on this last field, and give an overview of what is currently achievable and what may be possible in the future (my crystal ball permitting!).

Industry event (Wen, 16:30)

<u>NXP Semiconductors – Secure Connections for</u> <u>a Smarter World</u>: Dr. Alexander van Staa and Dr. Johanna Busch (NXP Semiconductors Germany GmbH, Hamburg, Germany)

"Isn't that the semiconductor company? What exactly do they do?" Get yourself more familiar with NXP Semiconductors in a brief presentation about the company, its business units and exciting possibilities for Graduates!

NXP Semiconductors enables secure connections and infrastructure for a smarter world, advancing solutions that make lives easier, better and safer. As the world leader in secure connectivity solutions for embedded applications, we are driving innovation in the secure connected vehicle, end-toend security & privacy and smart connected solutions markets.

The business units Automotive and Security & Connectivity are located in Hamburg. NXP's Automotive business unit offers sensor and processing technology that drives all aspects of the secure connected cars of today and the autonomous cars of tomorrow. NXP's Security & Connectivity business unit offers best-in-class security, contactless performance and the most complete solutions to produce unmatched mobile and Internet of Things (IoT) solutions.

NXP Semiconductors offers exciting possibilities for Graduates e.g. the Trainee Programs in Hamburg for technical and commercial roles embedded in a 2-year-program, comprising high-impact work in important projects, technical and professional training and ongoing exchange with top colleagues from around the world.

Practical information

Location

Campus Bahrenfeld

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

- Center for Free-Electron Laser Science (CFEL), Building 99
- Zentrum f
 ür Optische Quantentechnologien (ZOQ), Building 90

Physics Department Jungiusstraße 9

- Pool room 1 No. 306 3rd floor
- Pool room 3 No. 302, 3rd floor

<u>Contact</u>

Jutta Voigtmann Universität Hamburg, Bahrenfeld campus, Bld. 61 Luruper Chaussee 149 22761 Hamburg Phone: +49 40 8998 6696 E-mail: <u>cui.office@cui.uni-hamburg.de</u>

Dr. Antonio Negretti Universität Hamburg, ZOQ, Bld. 90, Room 104 Luruper Chaussee 149 22761 Hamburg Phone: +49 40 8998 6504 E-mail: <u>anegrett@physnet.uni-hamburg.de</u>

<u>Registration</u>

The registration to the graduate days takes place on Monday, March 13, 2017, in the foyer of the CFEL (Bld. 99) from 08:30 to 09:20. All registered participants and invited speakers will be provided with a badge and meal vouchers.

Lunch and group photo

The common lunches will take place at the Desycanteen (Bld. 09) from 12:45 to 13:50. A group photo of all participants of the graduate days as well as of the invited speakers is scheduled for Tuesday, March 14, 2017, at 12:40. All participants meet in the foyer of the CFEL (Bld. 99).

Lab tours

Time-resolved crystallography

Meeting point: CFEL Foyer (CFEL Café) Contact: Marta Sans Valls

Quantum condensed-matter dynamics

Meeting point: CFEL Foyer (information desk) Contact: Daniele Nicoletti

Controlled molecule imaging

Meeting point: CFEL Foyer (entrance of seminar room I) Contact: Daniel Horke and Sebastian Trippel

Structure and dynamics of cold and controlled molecules

Meeting point: Foyer, building 67 Contact: Sergio Domingos, Sabrina Zinn, Benjamin Arenas

Femto BEC: Combining ultrafast physics with ultracold quantum matter

Meeting point: ZOQ Foyer Contact: Philipp Wessels

Quantum matter

Meeting point: ILP Foyer Contact: Henning Moritz

Solid-state laser

Meeting point: ILP Foyer Contact: Daniel-Timo Marzahl

Coherent x-ray scattering

Meeting point: Entrance of building 25f (ground floor) Contact: Joana Valerio

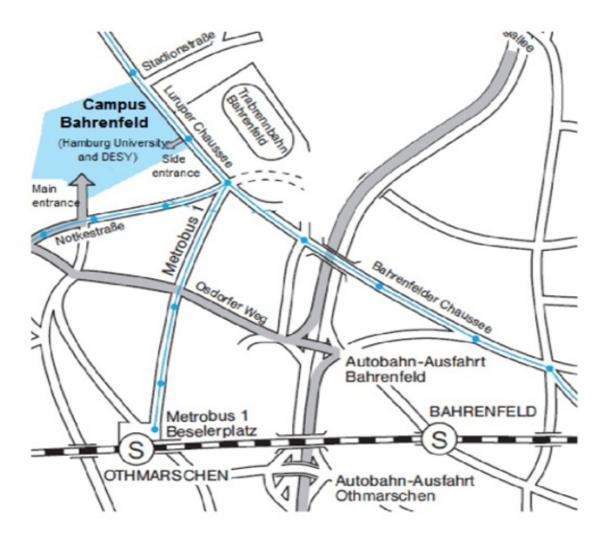
Biochemistry and molecular biology

Meeting point: Seminar room, building 22a (1st floor) Contact: Markus Perbandt

Petra III

Meeting point: Main entrance of PETRA III building 47c Contact: Oliver Seek

Directions

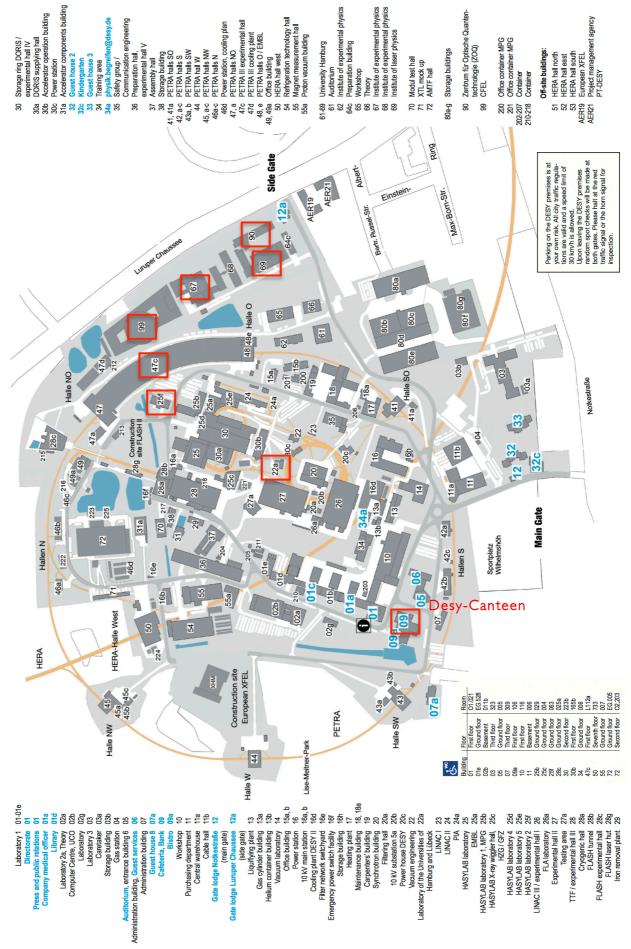


By train: to Hamburg-Altona station, then continue by taxi (travelling time about 15 minutes) or take a bus (see below).

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 I (direction "Schenefelder Holt") 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).



September 2012

Directions

From Dammtor station (public transport timetables on www.hvv.de) to the Physics Department

Exit Dammtor station: direction taxi rank. Turn West on Dag-Hammarskjöld-Platz. Pass the Radisson Blu on your right side. Enter the garden Planten and Blomen and follow the path (glass roofing) toward the Hamburg fair. At the end turn left. Cross Marseiller Strasse toward Jungiusstrasse. Cross again the Jungiusstrasse. Please enter Jungiusstraße 9, 3rd floor.

