

***The Hamburg Centre for Ultrafast Imaging
The Graduate Days 2016***

Hamburg
March 14 – 17

Programme

Monday, March 14, 2016

- 8:30** Registration (CFEL, Bld. 99, Foyer)
- 9:30** **Dr. Iacopo Carusotto**
Quantum fluids of light
(CFEL, Bld. 99, Seminar Room III, ground floor)
- Dr. Jan Helbing**
Ultrafast dynamics in the liquid phase – Spectroscopic methods and (bio-)chemical examples
(CFEL, Bld. 99, Seminar Room I, ground floor)
- Prof. Stephan W. Haas**
Phase transitions in low-dimensional systems
(ILP, Bld. 69, Seminar Room, ground floor)
- 10:50** Coffee Break (CFEL, ILP)
- 11:10** **Dr. Iacopo Carusotto**
Quantum fluids of light
(CFEL, Bld. 99, Seminar Room III, ground floor)
- Dr. Jan Helbing**
Ultrafast dynamics in the liquid phase – Spectroscopic methods and (bio-)chemical examples
(CFEL, Bld. 99, Seminar Room I, ground floor)
- Prof. Stephan W. Haas**
Phase transitions in low-dimensional systems
(ILP, Bld. 69, Seminar Room, ground floor)
- 12:30** Lunch (DESY Canteen, Bld. 09)
- 14:00** **Dr. Mathieu Le Tacon**
Introduction to lattice dynamics, charge, magnetic, and orbital excitations in complex matter
(CFEL, Bld. 99, Seminar Room III, ground floor)
- Dr. Jocelyne Vreede**
Molecular simulation of biomolecules
(CFEL, Bld. 99, Seminar Room I, ground floor)

Prof. Dmitri V. Talapin
Nanocrystal assemblies: A modular approach to materials design
(ILP, Bld. 69, Seminar Room, ground floor)

15:30 Free time

16:30 Lab tours

Tuesday, March 15, 2016

- 9:30** **Dr. Iacopo Carusotto**
Quantum fluids of light
(CFEL, Bld. 99, Seminar Room III, ground floor)
- Dr. Jan Helbing**
Ultrafast dynamics in the liquid phase – Spectroscopic methods and (bio-)chemical examples
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(ILP, Bld. 69, Seminar Room, ground floor)

15:30 Coffee Break (CFEL, ILP)

16:30 Colloquium

Prof. Boris Altshuler

Historical review of Anderson localization
(CFEL, Bld. 99, Seminar Rooms I-II-III)

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

Wednesday, March 16, 2016

9:30 Dr. Iacopo Carusotto

Quantum fluids of light
(CFEL, Bld. 99, Seminar Room III, ground floor)

Dr. Jan Helbing

Ultrafast dynamics in the liquid phase – Spectroscopic methods and (bio-)chemical examples
(CFEL, Bld. 99, Seminar Room I, ground floor)

Prof. Stephan W. Haas

Phase transitions in low-dimensional systems
(ILP, Bld. 69, Seminar Room, ground floor)

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11:10 Dr. Iacopo Carusotto

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15:30 Coffee Break (CFEL, ILP)

16:30 Industry event

Dr. Robert Riedel and Dr. Solveig Moré

How to turn your innovations to money and how to protect them
(CFEL, Bld. 99, Seminar Rooms I-II-III)

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

Thursday, March 17, 2016

9:30 Bernd Klein

Introduction into Python for scientists and engineers
(Physics Department, Jungiusstr. 9, 20355 Hamburg, Pool Room 3 – No. 302, 3rd floor)

Bodo P. Krause-Kyora

Introduction into Cuda
(Physics Department, Jungiusstr. 9, 20355 Hamburg, Pool Room 1 – No. 306, 3rd floor)

Rob Thompson

Communication – Negotiate - Resolve
(Bahrenfeld Campus, ILP, Bld. 69, Seminar Room 203, 2nd floor)

Monica Schofield

Start-up I: Is it for you? Developing business ideas from your own research
In cooperation with the PIER Helmholtz Graduate School
(Bahrenfeld Campus, CFEL, Bld. 99, Seminar Room IV, 1st floor)

Dr. Margarethe Remmert-Rieper

*Start-up II: Setting up your own company.
How to implement a successful business*
In cooperation with the PIER Helmholtz
Graduate School
(Bahrenfeld Campus, CFEL, Bld. 99,
Seminar Room V, 1st floor)

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12:30 Lunch (DESY Canteen, Bld. 09 or Bucerius
Law School Canteen, Jungiusstr. 6, 20355
Hamburg)

14:00 Bernd Klein

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Introduction into Cuda
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15:20 Coffee Break (CFEL, ILP, 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)

Quantum fluids of light: Dr. Iacopo Carusotto (INO-CNR BEC Center and University of Trento, Trento, Italy)

In these lectures I will introduce the audience to the physics of fluids of many interacting photons, a field that is presently experiencing impressing developments.

In suitable photonic devices, photons acquire a finite mass due to confinement and diffraction and significant binary interactions arise from the optical nonlinearity of the medium. As a result, a light field composed of many photon can display collective behaviours as a fluid.

After a short review of basic concepts of statistical mechanics and many-body physics, I will discuss the main experimental achievements of this field, trying to highlight the novel features as compared to more traditional systems such as liquid helium, electron gases, and ultracold atoms. A special attention will be given to Bose-Einstein condensation and superfluidity effects.

In the last part of the course, I will briefly sketch two among the most active axes of present research in this field, namely the quest for strongly correlated many-photon states in strongly nonlinear media and the realization of the so-called synthetic magnetic fields for photons. The combination of these two ideas is expected to open exciting new perspectives in the direction of mastering topological quantum effects with strong potential technological applications to quantum photonics.

Ultrafast dynamics in the liquid phase – Spectroscopic methods and (bio-)chemical examples: Dr. Jan Helbing (University of Zurich, Zurich, Switzerland)

The development of time-resolved X-ray and electron diffraction and imaging techniques brings us closer to the dream of directly observing structure during chemical reactions with atomic resolution. However, almost everything we know to date about ultrafast processes in molecules and their environment is derived from more indirect

spectroscopic observations in the UV-visible and infrared spectral range.

In this lecture we will focus on such experiments, which probe the electronic and vibrational response of isotropic (liquid) samples. There will be an emphasis on modern methods with enhanced information content and sensitivity. I plan to cover the following topics:

- A brief classification of non-linear spectroscopies: response theory and correlation functions
- Pump-probe and beyond: typical problems addressed with two and more laser pulses
- Photo-triggers: methods for initializing fast (bio)-chemical processes
- Intrinsic and artificial spectroscopic labels for probing structural change, electron and energy flow
- Polarization spectroscopy: time-dependent angle information in isotropic samples
- Multidimensional spectroscopies: experimental implementations, information content and common applications

Phase transitions in low-dimensional systems: Prof. Stephan W. Haas (University of Southern California, Los Angeles, USA)

In this lecture series, we will gain familiarity with the modern theory of phase transitions applied to classical and quantum systems, such as the Ising model. Using practical examples, we will learn how to develop and apply scaling theory, extract critical exponents, and thus identify fixed points associated with phase transitions. We will cover a range of numerical and theoretical approaches, including exact diagonalization, Monte Carlo, mean field theory and the renormalization group.

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

Introduction to lattice dynamics, charge, magnetic, and orbital excitations in complex matter: Dr. Mathieu Le Tacon (Max Planck Institute for Solid State Research, Stuttgart, Germany)

The design of new materials with tailored electronic properties, in analogy with what has been achieved for semiconductors last century, is currently at the forefront of condensed matter and material science research. A large effort focuses on materials in which electrons are strongly interacting with each other, and that challenge the standard quantum theory of solids. In these materials, new, unforeseen, states of electronic matter (e.g. colossal magneto-resistance, metal-insulator transition, giant thermopower, interface superconductivity, electronic Nematicity, Multiferroicity, density waves etc...) are experimentally observed.

Their macroscopic, thermodynamic, properties that is, their ability to exchange energy or entropy with the rest of the universe, are ultimately determined by the set of possible excited states they can reach from their ground state. As such, understanding the elementary excitation spectra of these materials and the interplay between these excitations, is the key to unveil the details of the interactions at the microscopic level, and a necessary step towards the control and the manipulation of the electronic properties of this quantum mater.

These can be excitations can be of different kind: from the crystal lattice, or from the electronic degrees of freedom (e.g. charge, spin or orbital). In these lectures, I will discuss some of the investigation tools that are used to probe such excitations. Special emphasis will be made on photon (from visible to hard x-rays) and neutron scattering methods, as well as on the recent developments that allows the investigation of materials under extreme temperature, pressures or magnetic fields environments.

Molecular simulation of biomolecules: Dr. Jocelyne Vreede (University of Amsterdam, Amsterdam, The Netherlands)

1) Molecular Dynamics

Protein behavior is fundamentally governed by intra- and intermolecular forces and often driven by thermal fluctuations [1]; therefore, a theoretical description naturally requires the language of statistical thermodynamics. Hence, molecular

simulations are the computational tool of choice. In particular, the advent of molecular dynamics (MD) simulation [2] and the development of appropriate interaction potentials, a.k.a. force fields, for biomolecules have had an enormous impact (see, for instance, Ref. [3]). When bond breaking and making is not required, classical force fields can describe the dynamics of proteins. Reasonably accurate atomistic classical force fields have been developed for proteins, and, while not perfect, provide an accurate description of many structural and dynamical properties of proteins [4]. In this lecture I will derive basic molecular dynamics algorithms and expressions for interatomic interactions, for use in a force field. Furthermore, I will provide examples of using force field molecular dynamics to study conformational changes in proteins.

2) Enhanced Sampling

When performing simulations of conformational changes in proteins, one of the crucial problems is that these changes are often rare and occur on the millisecond to second timescale. Such time scales are not accessible for all-atom MD simulations even on today's fastest computers, maybe with the exception of D.E. Shaw's Anton computer [4]. Rare events are usually related to the existence of high free energy barriers or entropic bottlenecks partitioning the configuration space of the system in different metastable basins (e.g. the folded and unfolded region in a protein). Hence, knowledge of the (free) energy landscape is of crucial importance to understand conformational transitions. Such a landscape also directly yields equilibrium behavior e.g. equilibrium constants, which can be compared to experiment. One method to explore protein free energy landscapes is the metadynamics technique [5]. In a predefined multidimensional space of collective variables, the method employs a history dependent potential that is augmented regularly with a Gaussian potential at the current position of the system. This way system is slowly pushed out of a free energy minimum and forced to explore other parts of configuration space. A disadvantage of metadynamics is that finding the correct conformational space heavily depends on the choice of the collective variables. The replica exchange molecular dynamics (REMD), also known as parallel tempering, does not suffer from this problem. In REMD, many MD replicas run simultaneously in parallel, at different temperatures [2,6]. By letting the replicas exchange temperatures, a system can diffuse through temperature space and overcome barriers at high temperature, while sampling the interesting stable states at the temperature of interest. Afterwards, the free energy can be obtained by constructing a histogram along

any order parameter. In this lecture I will discuss the background of the metadynamics and replica exchange MD methodologies, illustrated with relevant examples.

3) Sampling Rare Events

Free energy methods, such as metadynamics, are very useful for the computation of equilibrium constants and thermodynamic properties, but are less suitable for finding reaction mechanisms or rate constants of rare events. The classical way to calculate the rate constant is described by the transition state theory (TST). In TST the rate is approximated by the exponential of the activation free energy (i.e. the maximum of the free energy barrier along the reaction coordinate) and a kinetic prefactor. The Bennett-Chandler algorithm for dynamical corrections to TST provides an in principle exact route for the calculation of reaction rate constants [7, 8]. The applicability of transition state theory relies on the knowledge of an appropriate reaction coordinate. A reaction coordinate is a function of the configurational degrees of freedom of the system and should be capable of characterizing the progress of a transition through the dynamical bottleneck region. If the reaction coordinates are chosen in a way that does not capture the essential mechanisms involved in the transition, both TST and the Bennett-Chandler method fail. The transition path sampling (TPS) method harvests ensembles of unbiased dynamical trajectories between stable states by importance sampling [9,10]. The main advantage of the path sampling methodology is that it creates unbiased dynamical trajectories of the process of interest without knowledge of the reaction coordinate, while still bypassing the enormous waiting time in stable states. The path sampling method is a universally applicable importance sampling technique that has been successfully applied to many activated rare event processes, including protein folding, and protein conformational changes. See for a review [11]. In this lecture I will discuss transition state theory and transition path sampling, illustrated by examples on protein folding and protein conformational changes.

[1] Fersht, A. Structure and Mechanism in Protein Science, (Freeman, New York, 1999).

[2] D. Frenkel and B. Smit, Understanding molecular simulation, 2nd ed. (Academic Press, San Diego, CA, 2002).

[3] Karplus, M. "Special issue on: Molecular Dynamics Simulation of Biomolecules" edited by Martin Karplus, Acc. Chem. Res. 35 (2002).

[4] Lindorff-Larsen, K. et al., Science 334:517 (2011).

[5] A. Laio and M. Parrinello, Proc. Natl. Acad. Sci.

USA 99, 12562 (2002).

[6] Y. Sugita, and Y. Okamoto, Chem. Phys. Lett. 314, 141 (1999).

[7] Bennett, C.H. in Algorithms for Chemical Computations, ACS Symposium Series No. 46, edited by R. Christofferson (American Chemical Society, Washington, D.C., 1977).

[8] Chandler, D.J. Chem. Phys. 68:2959 (1978).

[9] Dellago, C., et al. J. Chem. Phys. 108:1964 (1998).

[10] Bolhuis, P.G., et al. Ann. Rev. Phys. Chem. 53:291 (2002)

[11] J. Juraszek, J. Vree de and P.G. Bolhuis, Transition path sampling of protein conformational changes, Chem. Phys. (2012) 396:30

Nanocrystal assemblies: A modular approach to materials design: Prof. Dmitri V. Talapin (The University of Chicago, Chicago, USA)

This lecture series will discuss modern approaches to the bottom-up design of functional materials from nanoscale building blocks, with some emphasis on semiconductor nanostructures and their applications for electronics and optoelectronics.

1. Synthesis and surface science of inorganic nanocrystals

Development of synthetic methods for well-defined nanostructures has introduced new route for engineering functional materials via synthesis and assembly of nano- and mesoscale building blocks. All nanomaterials share a common feature of large surface-to-volume ratio, making their surfaces the dominant player in many physical and chemical processes. Surface ligands, molecules that bind to the surface, are an essential component of size and shape control during the nanomaterial synthesis, processing, and application. Understanding structure and properties of nanoscale interfaces requires an intricate mix of concepts and techniques borrowed from surface science and coordination chemistry. I will elaborate these connections and discuss the bonding, electronic structure and chemical transformations at nanomaterial surfaces.

2. Self-organization of nanoscale building blocks: the role of size, shape and interactions

Nanoparticles of different functional materials can self-assemble from colloidal solutions into long range ordered periodic structures (superlattices). Such assemblies provide a powerful platform for designing macroscopic solids with tailored electronic, magnetic, optical and catalytic properties. Unlike atomic and molecular crystals where atoms, lattice geometry, and interatomic distances are fixed entities, the arrays of

nanocrystals represent solids made of “designer atoms” with potential for continuous tuning their physical and chemical properties.

The self-assembly process is guided by an intricate interplay of entropy-driven crystallization and soft interparticle interactions, such as van der Waals and dipolar forces. On the example of tetrahedral CdSe nanocrystals, I will show that non spherical shape introduces rotational entropy as an important additional term to the free energy balance. The surface ligands also play an important and sometimes counterintuitive role, supporting many-body interactions and stabilizing complex structures.

3. Application-targeted design of nano- and mesostructured materials

The nanocrystal assemblies offer an appealing manufacturing strategy that combines advantages of crystalline inorganic semiconductors with inexpensive solution-based device fabrication. Semiconductor nanocrystals are explored as the functional elements in commercial TVs and displays, printable electronics, light emitting devices, photodetectors and solar cells. Many of these applications rely on efficient injection, extraction and transport of charge carriers. By using optimized surface chemistries, nanocrystal arrays can exhibit carrier mobilities comparable to single crystal semiconductors. I will demonstrate the power of “modular” materials fabrication for electronic, thermoelectric and photovoltaic devices. For example, modular materials can be used for solution processed field-effect transistors with electron mobility over $300 \text{ cm}^2/\text{Vs}$, and for solar cells with the power conversion efficiency over 13%, all achieved through rational assembly of surface-engineered nanoscale building blocks. These and other examples demonstrate the utility of engineered nanomaterials for real-world technologies and applications.

Practical information

Location

Campus Bahrenfeld

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

- Center for Free-Electron Laser Science (CFEL), Building 99
- Zentrum für Optische Quantentechnologien (ZOQ), Building 90
- Institut für Laserphysik (ILP), Building 69

Seminar rooms IV and V in the CFEL are located on the first floor. The seminar room 203 in the ILP is located on the second floor. All other rooms are located on the ground floor.

Physics department

Jungiusstraße 9

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

Contact

Jutta Voigtmann

Universität Hamburg, Bahrenfeld campus, Bld. 61

Luruper Chaussee 149

22761 Hamburg

Phone: +49-40-8998-6696

E-mail: cui.office@cui.uni-hamburg.de

Dr. Antonio Negretti

Universität Hamburg, ZOQ, Bld. 90, Room 104

Luruper Chaussee 149

22761 Hamburg

Phone: +49-40-8998-6504

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

Registration

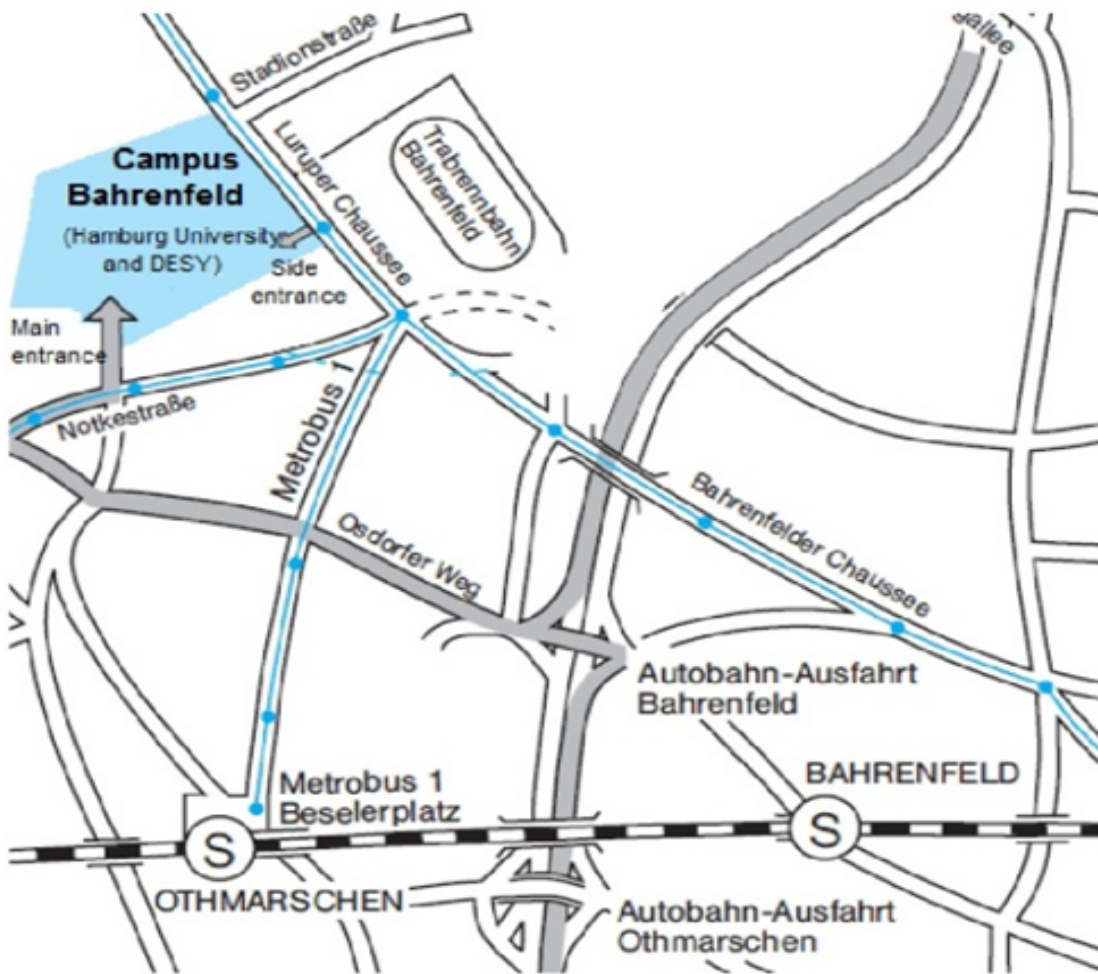
The registration to the Graduate Days takes place on Monday, March 14, 2016, in the foyer of the CFEL (Bld. 99) from 08:30 to 09:20 am. All registered participants and invited speakers will be provided with a badge and meal vouchers.

Lunch and group photo

The common lunches from Monday to Wednesday will take place at the DESY Canteen (Bld. 09) from 12:45 to 13:50. On Thursday, March 17, 2016, the lunch will also take place in the Bucerius Law School Canteen, Jungiusstr. 6, 20355 Hamburg.

A group photo of all participants of the Graduate Days as well as of the invited speakers is scheduled for Tuesday, March 15, 2016, at 12:40. All participants meet in the foyer of the CFEL (Bld. 99).

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 “Schenefelder Holt” or “Rissen”) 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).

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 Marseller Strasse toward Jungiusstrasse. Cross again the Jungiusstrasse. Please enter Jungiusstrasse 9, 3rd floor.

