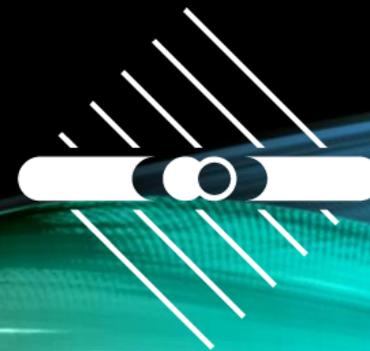


SOFT MATTER meets ULTRAFAST SPECTROSCOPY SMUS2020

Online Workshop

31st August – 1st September 2020

MAX PLANCK
GESELLSCHAFT



cost
EUROPEAN COOPERATION
IN SCIENCE & TECHNOLOGY



MAX-PLANCK-INSTITUT
FÜR KERNPHYSIK

AttoChem
Attosecond Chemistry

GOALS

- Gather international scientists from complementary disciplines with the aim to achieve a deeper understanding of the electronic and nuclear dynamics occurring at an extremely wide temporal and spatial scale in LCs, and more generally in soft matter from both experimental and theoretical point of view.
- Present broad overview about current hot topics in research activities of soft matter thus liquid crystals, ultrafast spectroscopy techniques such as THz, transient absorption or high harmonic generation spectroscopy, and computational tools to capture such dynamics.
- Formation of an initial network which will prepare the ground for future joint research activities and establish new collaborations among scientists working in liquid crystals (soft matter) and ultrafast dynamics from both theoretical and experimental point of view.
- Exchange of students/ early career scientists (PhD and postdocs) allowing knowledge transfer across collaborating research groups.

SESSIONS

- **Current research on Liquid Crystal & Soft Matter: Latest frontiers on material design and theory**
- **Ultrafast dynamics in condensed matter and large molecular systems: preparing the ground for Liquid Crystal ultrafast investigation**
- **AttoChem WG3 session: Towards Attosecond chemistry of Liquid Crystal**

INVITED PEOPLE

4

Invited speaker	Research activity
Prof. Paul Kouwer:	Synthesis of soft matter based materials and their structural properties such as hydrogels and different types of liquid crystals.
Prof. Miha Ravnik:	Modeling and simulation of soft and partially ordered matter from macroscopic phenomenology to microscopic molecular modeling.
Prof. Marco Mazza:	Modelling and simulation of nonequilibrium systems: from microorganisms forming biofilms, or flocks of birds self-organizing, to nonequilibrium transitions in granular material.
Prof. Steven Johnson:	Nonlinear dynamics of the atomic structure in solid-state materials.
Prof. Francesca Calegari:	Attosecond ultrafast dynamics in systems with increasing complexity from simple molecules to molecules of biological interest and nanostructured materials.
Dr. Christian Ott:	Attosecond strong field physics in atomic and molecular systems.
Prof. Milutin Kovacev:	High-level research on pulsed lasers and their application from the shortest pulses with single cycle durations via high repetition rate high-energy sources to terawatt peak powers.
Prof. Fernando Martin:	Theoretical study of the dynamics in isolated quantum systems, from atoms to extended systems, as in the interaction of molecules with metallic surfaces with ultrashort laser pulses.
Prof. Angel Rubio:	Modeling and theory of electronic and structural properties of condensed matter.
Prof. Herma Kuppen:	Computational chemistry in organic crystals.
Dr. Hanieh Fattahi:	Femtosecond fieldoscopy.

PROGRAM⁵

	Day 1_Monday August 31 st	Day 2_Tuesday September 1 st
9:00 start	Introduction day 1 - Cattaneo	Introduction day 2 - Cattaneo
9:15	Kower: Challenges in soft matter materials: from responsive to autonomous	Mazza: Liquid crystals out of equilibrium
9:45	Ravnik: Modelling of flow of light in nematic birefringent structures	Kuppen: TBA
10:15	Rubio: QED-materials and Floquet engineering	Fattahi: Near-Infrared Molecular Fieldoscopy
10:45	PAUSE	PAUSE
11:00	Johnson: Linear and nonlinear THz spectroscopy of solids	Kovacev: High-Harmonic Generation from liquid water droplets
11:30	Calegari: Tracking electron dynamics in bio-chemically relevant molecules	Martin: Imaging and controlling electron molecular dynamics: towards attochemistry
12:00	PAUSE	PAUSE
12:15	Ott: The strong-field-driven dipole response in complex systems: Resolving laser-driven femtosecond and attosecond coherent dynamics	Place for new contributions and/or discussion
12:45	Conclusive thoughts - Cattaneo	Conclusive thoughts - Cattaneo
13:00 end		



TITLES AND ABSTRACTS

PAUL KOUWER

Challenges in soft matter materials: from responsive to autonomous

Materials in biology are not static but show a large temporal and also spatial variation. For instance, the cells continuously change their microenvironment by depositing and degrading components in their surrounding matrix, thereby always controlling the properties.

Currently in synthetic materials, there is a strong drive towards responsive materials that change their properties after the application of an (external) stimulus. Can we take the next step to generate materials that change properties after a cellular cue or even autonomously?

MIHA RAVNIK

Modelling of flow of light in nematic birefringent structures

Complex nematic fluids allow for creation or self-assembly of various birefringent structures, which can be used for micro-manipulate the flow of light. Here, we show selected examples of modelling the flow of light in selected nematic birefringent structures, including their performance as cloaking devices, photonic crystals, lasers, and metamaterials. Methodologically, we use numerical modelling based on custom adapted solving of Maxwell's equations by (i) Finite Difference Time Domain (FDTD) simulations which can access dynamic fast scales, and (ii) Finite Difference Frequency Domain (FDFD) simulations which solve the light modes emergent in the birefringent profiles. More generally, the aim of this talk is to demonstrate the possible approaches to use birefringent nematic materials in beyond-the-display applications, crucially using different – orders of magnitude shorter- length and time scales.

MARCO MAZZA

Liquid crystals out of equilibrium

I will discuss some recent results on liquid crystals in nonequilibrium. First, hydrodynamic cavitation, the nucleation of vapour in liquids. With a combination of microfluidic experiments, nonequilibrium molecular dynamics simulations and theoretical arguments, we have studied flow-induced cavitation in a nematic fluid.

The cavitation domain nucleates due to sudden pressure drop upon flow past a cylindrical obstacle within a microchannel. For an anisotropic fluid, the inception and growth of the cavitation domain ensued in the Stokes regime, while no cavitation was observed in isotropic liquids flowing under similar hydrodynamic parameters.

Second, some ongoing work on the dynamics of active nematic droplets will be briefly discussed.

FRANCESCA CALEGARI

Tracking electron dynamics in bio-chemically relevant molecules

Attosecond science is nowadays a well-established research field, which offers formidable tools for the investigation and control of electronic processes. The possibility to study molecules of increasing complexity with attosecond time resolution paves the way to disclosing the role of the electron dynamics in the photo-chemistry and photo-biology of complex systems. In this context, I will provide a few examples of the observation of pure electron dynamics in biomolecular building blocks including amino acids and DNA nucleobases. I will then discuss possible approaches for the investigation of these complex molecules in their natural environment, i.e. in water.

CHRISTIAN OTT

The strong-field-driven dipole response in complex systems: Resolving laser-driven femtosecond and attosecond coherent dynamics

We use ultrashort XUV and few-cycle VIS/NIR optical pulses to probe the absorption spectra of moderately dense gas- and liquid-phase targets, respectively, in Fraunhofer-type transmission geometry. In the time domain, the ultrashort probing pulse triggers a dipole response that then further evolves in a field-free environment. It is this dipole response, emitted in forward direction, that interferes with the incoming pulse and gives rise to sharp spectral signatures in the measured absorption spectrum (i.e., spectral lines), despite extremely short pulses with much larger Fourier spectral bandwidth are being used. Benefitting from the use of time-synchronized ultrashort laser pulses it is possible to further modify this dipole response of the probe-excited system with a moderately strong laser field. Coherent control of the absorption line shapes can thus be achieved with access to both amplitude and phase, and the laser imprint on the time-dependent dipole response can be directly extracted from the measured spectra in real time, with sub-femtosecond temporal resolution. In this talk I will present experimental results on the real-time buildup dynamics of complex spectral structures encoded in the Rydberg series of overlapping autoionizing Fano resonances in helium. Furthermore, I will discuss first experimental results on a much more complex target, aluminum phthalocyanine chloride dissolved in ethanol, as an example for the coherent strong-field control of liquid-phase VIS absorption spectra.

STEVE JOHNSON

Linear and nonlinear THz spectroscopy of solids

I give a short overview of the current state of the art in THz spectroscopy of solids, with an emphasis on nonlinear optical effects in the THz regime and how they can be detected. I give some recent examples in correlated electron systems and discuss their possible wider applications in soft matter.

MILUTIN KOVACEV

High-Harmonic Generation from liquid water droplets

An overview will be given on the subject of strong-field interactions with liquid water droplets. We will present our experimental measurements and theoretical simulations. The talk will also address the historical development, current challenges and future perspectives.

FERNANDO MARTIN

Imaging and controlling electron molecular dynamics: towards attochemistry

Sudden excitation or ionization of a molecule by visible, UV or XUV light is usually followed by charge redistribution on a time scale ranging from hundreds attoseconds to a few-femtoseconds, which can be followed by fragmentation of the remaining molecular cation up to a few picoseconds. Such complex dynamics arises from the coherent superposition of electronic states covered by the broadband pulse and from rearrangements in the electronic structure of the molecular cation due to electron correlation. To investigate these ultrafast processes, attosecond pump-probe spectroscopies have been shown to be very valuable tools [1-9]. In this talk I will present the results of gas-phase molecular pump-probe experiments and theoretical simulations in which several molecules and solids are ionized and subsequently probed in order to obtain the complete electronic movie. I hope that these results will help to guide future experimental efforts in more complicated molecules, even in the liquid phase, and will open the door to the control of charge transfer [10]. These efforts should be accompanied by the development of new theoretical methods able to accurately describe the ionization continuum of molecules in the gas [11] and condensed phases.

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- [11] A. Palacios and F. Martín, *WIREs Comp. Mol. Sci.*, e1430 (2020).

HANIEH FATTAHI

Near-Infrared Molecular Fieldoscopy

Linear spectroscopy in near-infrared spectral range provides information on the molecular composition, structure, and conformation, affording tremendous potential for high-resolution, in-depth, label-free biological spectromicroscopy [1]. Broadband measurements in this spectral region have been carried out mainly in the frequency domain, which suffers from two limitations: i) the detection of small absorption differences is limited to the intensity noise of the source, and ii) the low detection dynamic range.

To mitigate above-mentioned limitations, we introduce the concept of molecular Fieldoscopy. In molecular Fieldoscopy, an ultrashort, phase-coherent pulse is used for molecular excitation and afterwards the transmitted complex electric field that contains the molecular response is measured directly. Here, the excitation pulse is confined to a time window of tens of femtoseconds, which is significantly shorter than molecular response. Therefore, the molecular response is detected free of background and the effect of the intensity noise of the source is eliminated. Furthermore, measuring the complex electric field allows for extracting the full spectral phase information of the molecular response, adding a new dimension to the gained spectroscopic data.

1 F. F. Jöbsis, "Noninvasive, infrared monitoring of cerebral and myocardial oxygen sufficiency and circulatory parameters." *Science* 198, 1264–1267 (1977).

ANGEL RUBIO

TBA

HERMA KUPPEN

TBA

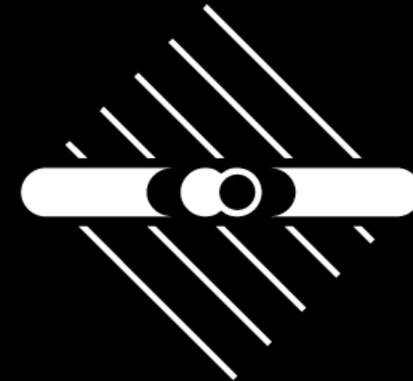
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- Prof. Angel Rubio: Max Planck Institute for the Structure and Dynamics of Matter (Hamburg, DE)
- Prof. Francesca Calegari: DESY (Hamburg, DE)
- Prof. Paul Kower: Radboud University (Nijmegen, NH)
- Prof. Steven Johnson: ETH Zurich (CH)
- Prof. Milutin Kovacev: Leibniz Universität (Hannover, DE)
- Dr. Hanieh Fattahi: Max Planck Institute for the Science of Light (Erlangen, DE)
- Dr. Christian Ott: Max Planck Institute for Nuclear Physics (Heidelberg, DE)

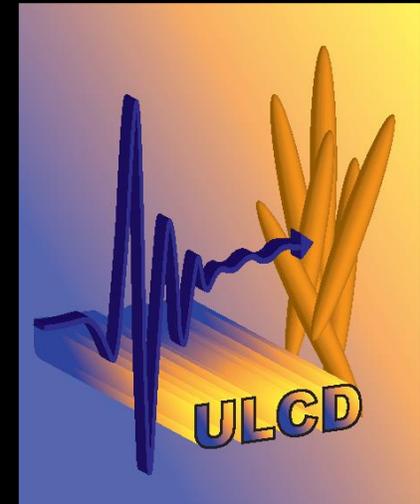
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