Mini-Workshop on “Advanced Spectroscopy of Molecules and Materials”

It is our pleasure to announce a mini-workshop on advanced spectroscopy of molecules and materials. The workshop aims to cover such hot topics of atomic, molecular and condensed matter physics as attosecond dynamics and topology.

Date: October 26
Time: 10:45-13:00
Room: HG00.616

10:45 Welcome Alexey Kimel/Theo Rasing

10:50-11:20 Laura Cattaneo (ETH, Zuerich). **Photoemission dynamics from atomic and molecular systems in attosecond timescale**

11:20-11:50 Oleg Tretiakov (Tohoku University, Sendai). **Skyrmions in ferromagnets and antiferromagnets**

11:50-12:20 Roman V. Pisarev (Ioffe Institute, St. Petersburg). **Electronic structure, magnetic phase transitions and optical phenomena in a complex magnetoelectric antiferromagnet CuB_2O_4**

12:20-12:50 Fulvio Parmigiani (Elettra-Sincrotrone Trieste, Trieste). **Science driven requirements for seeded soft X-ray free electron lasers**

At 15:45 in the Aula Alexey Kimel will give his inaugural lecture “Magnetism of light: a key to terra incognita”

Photoemission dynamics from atomic and molecular systems in attosecond timescale

Laura Cattaneo
ETH, Zürich, Switzerland

The recent progress in the creation of ultrashort light pulses has enabled the determination of photoionization time delays with attosecond precision. Pump-probe techniques, employing an extreme ultraviolet (XUV) attosecond pulse as pump and an infrared (IR) pulse as probe have become standard tools in attosecond science to determine relative timing information between electrons originating from different states within the same atom, different atoms or molecules. Thanks to the possibility to tune the XUV pulse length and structure, passing from an attosecond pulse train (APT) to a single attosecond pulse (SAP), we were able to perform a thorough comparison study of the most established techniques in the attosecond field, i.e. RABBITT and streaking [1]. In addition, by exploiting the photoelectron-ion coincidence detection and the full 3D momenta reconstruction, we can acquire angular resolved photoelectron- and ion-distributions to shed light on molecular photoionization time delays. In particular, I will present the dissociative photoionization of CO where we disentangle the contribution from different states, and the influence of double excited states on the photoemission time delays in H2.

[1]. L. Cattaneo *et al.,* "Comparison of attosecond streaking and RABBITT," Opt. Express **24**, 29060 (2016).

Skyrmions in Ferromagnets and Antiferromagnets

Tohoku University, Sendai, Japan

Skyrmions are topologically protected spin textures, which can be used in spintronic devices for information storage and processing. However, skyrmions in ferromagnets have some intrinsic difficulties, which must be overcome to use them for spintronic applications, such as the inability to move along electric current due to skyrmion Hall effect. It has been demonstrated that skyrmions can also be stabilized and manipulated in antiferromagnetic materials. An antiferromagnetic skyrmion is a composite topological object with a similar but of opposite sign spin texture on each sublattice, which results in the absence of skyrmion Hall effect. I will discuss the lifetime and stability of antiferromagnetic skyrmions at a finite temperature on the basis of a two-dimensional Heisenberg exchange model with external magnetic field, uniaxial anisotropy, and Dzyaloshinskii-Moriya interaction. The results will be compared to the case of a ferromagnet by inverting the sign of the exchange constant. Furthermore, I will show that surprisingly the topological spin Hall effect of antiferromagnetic skyrmion texture is nonzero and enhances the spin transfer torques acting on the skyrmion.

Electronic structure, magnetic phase transitions and optical phenomena in a complex magnetoelectric antiferromagnet CuB_2O_4

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During the last decade, the magnetic and optical properties of copper metaborate CuB_2O_4 became a subject of active and sometimes controversial research. It has a complex non-centrosymmetric crystal structure *-42m* (*Z*=12) in which magnetic Cu^{2+} ions (*S*=1/2) occupy 4*b* and 8*d* distinct positions. 4*b* subsystem orders antiferromagnetically at T_{N1}=21 K, whereas 8*d* subsystem becomes partly ordered below T_{N2}~9 K. CuB_2O_4 possesses unique optical properties [1-3]. Six anomalously narrow zero-phonon (ZP) lines were observed at low temperatures, each of them being accompanied by broad phonon sidebands with well resolved structure (see Fig. 1). These features in the spectral range of 1.4-2.4 eV are due to electronic transitions between $3d^9$ states of Cu^{2+} ions in the crystal field. All six ZP lines show strong changes at the magnetic phase transitions. We have observed a strong linear dichroism relevant to ZP lines of the 4*b* subsystem for the light propagating along the optical axis. The dichroism appears below T_{N1}=21 K due to the ordering of the 4*b* spins in the (001) plane (see Fig. 2). A splitting of the magnetic phase transition near 9 K was observed for the first time. Below 6 K in the incommensurate phase we proposed a spin ordering different from previously suggested.

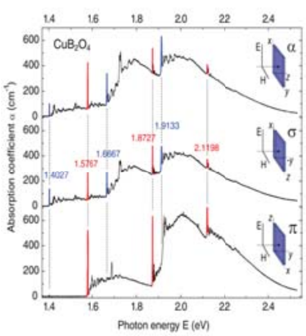

Fig. 1. Optical absorption spectra for three different α, σ and π polarizations [1].

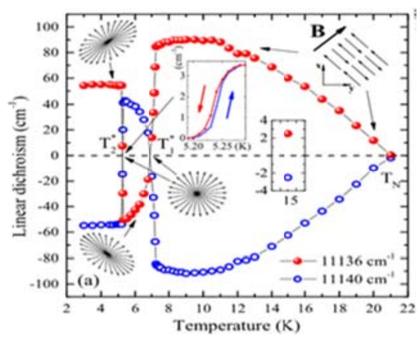

Fig. 2. Antiferromagnetic linear dichroism in the 4*b* subsystem as a function of temperature [2].

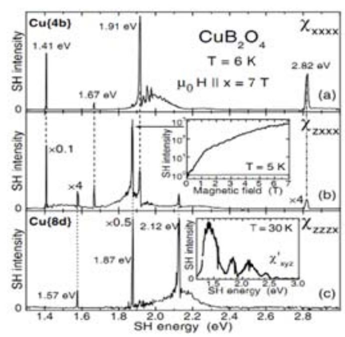

Fig. 3. SH generation spectra due to spin ordering in the 4*b* and 8*d* subsystems [3].

The crystal structure of CuB_2O_4 is non-centrosymmetric and therefore the optical second harmonic generation (SHG) is allowed. It was very challenging to see the coupling of SHG to magnetic properties of both sublattices. The study was performed in magnetic field up to 7 T applied along different crystal axes [3]. Fig. 2 shows the spectra of magnetic-field-induced SHG. The strongest SHG signals, as in the case of the linear dichroism, were observed at the ZP lines. Analysis of the results allowed us to clearly distinguish contributions from the 4*b* and 8*d* sublattices, their behavior in an applied magnetic field, and the relevant phase diagrams for each sublattice.

This work was supported by the Russian Science Foundation grant № 16-12-10456.

[1] R.V. Pisarev, A.M. Kalashnikova, O. Schöps, *et al*, *Phys. Rev. B* **84**, 075160 (2011).
[2] R.V. Pisarev, I. Sänger, G.A. Petrakovskii, *et al*, *Phys. Rev. Lett*. **93**, 037201 (2004).
[3] K.N. Boldyrev, R.V. Pisarev, L.N. Bezmaternykh, *et al*, *Phys. Rev. Lett*. **114**, 247210 (2015).

Science driven requirements for seeded soft X-ray free electron lasers

Fulvio Parmigiani

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Starting from the archetypal FERMI externally seeded FEL, recent theoretical and experimental progress has shown the possibility of producing fully coherent, variable polarization and tunable, soft-X-ray, ultra-short pulses at high repetition rate.

This ultimate achievement will unlock the gate for performing X-ray-based experiments that are qualitatively different from those available at any current or planned X-ray source.

Here we will review the experiments and the ideas that represent the science frontier in soft X-ray, time-resolved spectroscopy, coherent imaging and X-ray coherent optics non-equilibrium spectroscopy.

These studies will lead to an understanding of fundamental dynamics, occurring on the ultrafast time and nanometer spatial scales, needed for addressing a broad range of science essential for resolving our complex and long-term energy challenges, environmentally urgent questions and demanding problems in bioscience and novel materials.