



# **Time resolved structural studies Synergy and complementarity between ESRF and XFEL**

**ESRF Auditorium – Grenoble, France  
4 + 5 March 2019**

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- **Programme**
  - **Abstracts**
  - **List of participants**

# Monday 4 March 2019

08:00 - 08:30

Registration - ESRF Entrance Hall

## Session 1 – chaired by Michael Wulff and Matteo Levantino

|               |   |
|---------------|---|
| 08:30 - 08:50 | <b>Jean SUSINI</b> , Director of Research, ESRF Grenoble, France<br><i>Opening remarks</i>                              |
| 08:50 - 09:10 | <b>Serguei MOLODTSOV</b> , European XFEL, Schenefeld, Germany<br><i>European XFEL: Status and Research Applications</i> |
| 09:10 - 09:45 | <b>Christian BRESSLER</b> , XFEL Germany<br><i>MHz X-ray Experiments with SR and XFEL sources</i>                       |
| 09:45 - 10:15 | <b>Michael WULFF</b> , ESRF Grenoble, France<br><i>The ID09 beamline: history and visions for the future</i>            |
| 10:15 - 10:45 | Coffee break  |

## Session 2 – chaired by Christian Bressler

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| 10:45 - 11:35 | <b>Richard NEUTZE</b> , University of Gothenburg, Sweden<br><i>Time resolved diffraction and scattering studies of protein structural changes using XFEL and synchrotron radiation</i> |
| 11:35 - 12:00 | <b>Giorgio SCHIRO</b> , Institut de Biologie Structurale - Grenoble France<br><i>X-ray pulses for time-resolved experiments on photo-sensitive proteins</i>                            |
| 12:00 - 12:25 | <b>Sebastian WESTENHOFF</b> , University of Gothenburg, Sweden<br><i>Time-resolved WAXS reveals solution structural changes in photoreceptor proteins</i>                              |
| 12:30 - 13:30 | Lunch at ESRF on-site restaurant   |

## Session 3 – chaired by Anton Plech

|               |  |
|---------------|--|
| 14:00 - 14:50 | <b>Majed CHERGUI</b> , EPFL Lausanne, Switzerland<br><i>Structural dynamics of hemoproteins using synchrotron radiation and X-ray free electron lasers</i>                                       |
| 14:50 - 15:15 | <b>Kristoffer HALDRUP</b> , Technical University of Denmark<br><i>Unpacking energetics and dynamics in photoexcited transition-metal complexes with synchrotrons and XFELs</i>                   |
| 15:15 - 15:40 | <b>Qingyu KONG</b> , Synchrotron SOLEIL<br><i>Photochemical reaction dynamics of <math>Ru_3(CO)_{12}</math> studied by picosecond and femtosecond X-ray solution scattering at ESRF and LCLS</i> |
| 15:45 - 16:15 | Coffee break   |

## Session 4 – chaired by Robert Feidenhans'l

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|---------------|--|
| 16:15 - 16:40 | <b>Dmitry KHAKHULIN</b> , XFEL Hamburg, Germany<br><i>FXE instrument of the European XFEL: experimental capabilities and first results</i>               |
| 16:40 - 17:05 | <b>Matteo LEVANTINO</b> , ESRF Grenoble, France<br><i>Time-resolved structural studies at the ID09 beamline of the ESRF</i>                              |
| 17:05 - 17:30 | <b>Anton PLECH</b> , Karlsruhe Institut of Technology, Germany<br><i>Time-resolved nanoscience – between molecular kinetics and solid-state dynamics</i> |
| 17:30 - 17:55 | <b>Charles PEPIN</b> , CEA France<br><i>Time-resolved synchrotron XRD of shock compressed matter : the case study of Bi</i>                              |
| 17:55 - 18:20 | <b>Simone TECHERT</b> , DESY Hamburg, Germany<br><i>Studying complex chemical reactions at pulsed high-flux X-ray sources</i>                            |
| 19:00 - 21:00 | Dinner at the ESRF on-site restaurant  |

## Tuesday 5 March 2019

### Session 5 – chaired by Sylvain Ravy

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|---------------|---|
| 08:30 - 09:20 | <b>Shin-ichi ADACHI</b> , KEK Photon Factory, Japan<br><i>Complementarity of SR and XFEL sources for tracking chemical reactions in solution with ultrashort X-ray pulses</i> |
| 09:20 - 09:50 | <b>Martin NIELSEN</b> , Technical University of Denmark<br><i>Kinetics and dynamics in bi-metallic complexes in solutions</i>   |
| 09:50 - 10:15 | <b>Peter GAAL</b> , Universität Hamburg, Leibnitz-Institut für Kristallzüchtung, Berlin, Germany<br><i>Implementation of a high repetition and short pulse option at ID09</i> |
| 10:15 - 10:45 | Coffee break  |

### Session 6 – chaired by Maciej Lorenc

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| 10:45 - 11:10 | <b>Pieter GLATZEL</b> , ESRF Grenoble, France<br><i>Chemical information in X-ray emission spectroscopy</i>  |
| 11:10 - 11:35 | <b>Grigory SMOLENTSEV</b> , Paul Scherrer Institute, Switzerland<br><i>Excited state of Cu-based OLED material is probed with pump-probe XAS, XES and WAXS</i> |
| 11:35 - 12:00 | <b>Thomas PENFOLD</b> , Newcastle University, United Kingdom<br><i>Time-resolved X-ray Spectroscopy: from the nano to the femtosecond regimes</i>              |
| 12:00 - 13:00 | Buffet lunch in the Auditorium   |

### Session 7 – chaired by Martin Meedom Nielsen

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|---------------|---|
| 13:00 - 13:25 | <b>Maciej LORENC</b> , Université de Rennes, France<br><i>Multiscale dynamics studied with X-rays : from molecular switching to material transformation</i> |
| 13:25 - 13:50 | <b>Tim Brandt VAN DRIEL</b> , SLAC National Accelerator Laboratory, USA<br><i>Experiences from the LCLS</i>   |
| 13:50 - 14:15 | <b>Sylvain RAVY</b> , Université Paris-Sud, France<br><i>Charge-density waves at the femto- and picosecond timescale</i>                                    |
| 14:15 - 15:00 | <b>Roundtable discussion</b>  |

## Abstracts



# European XFEL: Status and Research Applications

Serguei Molodtsov

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The European X-ray Free Electron Laser (XFEL) is a new international research installation that is currently under construction and in large part in operation in the Hamburg area in Germany. The facility will generate new knowledge in almost all the technical and scientific disciplines that are shaping our daily life - including nanotechnology, medicine, pharmaceuticals, chemistry, materials science, power engineering and electronics. The ultra-high brilliance femtosecond X-ray flashes of coherent radiation are produced in a 3.4-kilometre long European XFEL facility. Most of it is housed in tunnels deep below ground. In its start-up configuration, the European XFEL will comprise 3 self-amplified spontaneous emission (SASE) light sources – undulators operating in energy ranges 3 - 25 keV (SASE 1 and SASE 2) and 0.25 - 3 keV (SASE 3), respectively. The world-unique feature of this XFEL is the possibility to provide up to 27.000 ultra-short flashes (3 - 100 fs) that makes the facility unique and perfectly suitable for a large variety of research applications that are going to be reviewed in this presentation.

# MHz X-Ray Experiments with SR and XFEL Sources

Gawelda, W., Galler, A, and Bressler C.

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Time-resolved x-ray experiments at synchrotrons at MHz repetition rates offers the possibility to record transient data with static signal quality [1]. A MHz laser system synchronized to the pulse structure of the storage ring permits to use the entire SR flux in a pump-probe experiment.

We will show case examples, where previous experiments, limited to the kHz repetition rate of the standard amplified Ti:Sa laser system, are significantly boosted, when utilizing fibre-based amplified laser systems.

Such experiments are also possible at European XFEL, whose pulse structure also includes MHz pulse repetition rates. Its superior average flux make it more useful for advanced x-ray tools, and SR experiments exploiting XAS, XES, RIXS, and X-Ray Raman Spectroscopy will be presented.

## References

[1] - A. Britz, T. Assefa, A. Galler, W. Gawelda, M. Diez, P. Zalden, D. Khakhulin, B. Fernandes, P. Gessler, H. Sotuodi, A. Beckmann, M. Harder, H. Yavas, C. Bressler  
J. Synchr. Rad. **23**, 1409-1423 (2016).

# The ID09 beamline: history and vision for the future

Levantino M., Kabanova V., Sander M. and Wulff, M.

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Filming the structure of proteins at work, with atomic resolution and nanosecond time resolution, was the driving force for the first scientists on ID09 when the beamline opened for user experiments in September 1994. In a very fruitful collaboration with Prof Keith Moffat, University of Chicago, a mechanical chopper was built that allowed to isolate single X-ray pulses from the storage ring. The first experiment was a Laue diffraction study of the photo detachment of CO from the Fe binding site in myoglobin. The detachment of CO is reversible and it was possible to collect complete data with the W70 wiggler from one crystal [1]. We observed how CO is captured, just after photo dissociation, in a cavity next to Fe for ten nanoseconds before it diffuses into solution. The time resolution of this first setup was 5 ns from the first nanosecond laser on the beamline.

The installation of the high-speed chopper from Julich in 1998 was big step forward since it allowed to select single pulses at 1 kHz from several filling modes of the storage ring. That greatly increased the time available for pump-probe experiments which was essential to gain more experience. A 1 kHz femtosecond laser followed in 1999 which pushed the time resolution of the setup to 100 ps. It marked the completion of the first picosecond pump-probe setup worldwide. The 1 kHz rep rate allowed new diffraction experiments with monochromatic beams to be done. The discovery of a photo driven phase transition in a molecular crystal was done with the 1 kHz setup [2].

Another milestone was the pink beam from the U17 in-vacuum undulator in 2001. The U17 produced a very intense quasi monochromatic beam with up to  $5 \times 10^9$  photon per pulse at 15-18 keV. The 250-fold gain intensity made it possible to study molecular reactions in solution at unprecedented spatial and temporal resolution [3]. We discovered that the signals from the change in structure of a molecule in solution is accompanied by hydrodynamic changes in the solvent, i.e. the change in temperature, pressure and density. The theoretical framework was developed by Savo Bratos and Rodolphe Vuilleumier at the Université Jussieu in Paris in collaboration with the beamline scientists [4-5].

The optics and choppers on ID09 are prepared for the Extremely Bright Source (EBS) with a new micro focusing mirror and new choppers that will increase the pump-probe frequency to 3 kHz. The low emittance of the EBS will make the undulator peaks narrower and many more experiments will be done with the pink beam. The intensity on the sample will increase by factors of 5-10 and the beam will be focused to 20  $\mu\text{m}$ .

X-ray emission spectroscopy(XES) will greatly benefit from the increase in flux and pump-probe frequency. The prospect for increasing the pump-probe frequency to 20 kHz will be discussed.

## References

- [1] V. Srajer et al., Science, vol 274, 1726-1729, 1996.
- [2] E. Collet et al., Science, vol 300, 612-615, 2003.
- [3] H. Ihee et al., Science, 309, 1223-1227, 2005.
- [4] A. Plech, PRL, vol 92, 125505, 1-4, 2004.
- [5] M. Wulff et al., Journal of Chemical Physics, 124, 34501-34513, 2006.

# Time resolved diffraction and scattering studies of protein structural changes using XFEL and synchrotron radiation

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Time-resolved X-ray scattering and X-ray diffraction has led to new insights into how protein structural changes are coupled to protein function across a number of fields. With the advent of time-resolved serial crystallography we expect that the field will grow to incorporate a broader domain of structural targets. I will provide a historical overview of the development of time-resolved Laue diffraction and time-resolved X-ray scattering from ID09 of the ESRF. I will then discuss the advantages of time-resolved serial crystallography which has been developed using XFEL radiation and is likely to also be applied using synchrotron radiation. Although I will try to illustrate points in a manner that reflects the contribution of many scientists within the field, my presentation will fall short of providing a comprehensive review. Where appropriate, I will emphasize our collaborative work on the light-driven proton pump bacteriorhodopsin to illustrate the sort of structural insights and new details that can emerge from these methods. In conclusion I will argue that I foresee a complementarity between XFEL and synchrotron radiation as the field develops into the future.

## References

- [1] R. Neutze, K. Moffat, Time-resolved structural studies at synchrotrons and X-ray free electron lasers: opportunities and challenges, *Curr. Opin. Struct. Biol.* **22**, 651-659 (2012).
- [2] Nango, E. et al., A three-dimensional movie of structural changes in bacteriorhodopsin. *Science* **354**, 1552-1557 (2016).
- [3] P. Nogly et al., Retinal isomerization in bacteriorhodopsin captured by a femtosecond x-ray laser. *Science* **361**, eaat0094 (2018).



# **X-ray pulses for time-resolved experiments on photo-sensitive proteins**

Giorgio Schiro

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Biological macromolecules are characterized by specific structural and dynamic features that are at the basis of their biological activity. Understanding macromolecular activity thus requires studying structural changes over time and on various time-scales down to the femto-chemistry regime. Complementary use of time-resolved X-ray scattering and diffraction at synchrotrons and XFELs permit tracking conformational changes in photo-sensitive proteins along a photo-induced reaction pathway from the sub-ps regime to the millisecond time scale. I will show results from recent studies of light-induced protein structural dynamics in fluorescent proteins, photoreceptors and photoactivated ligand-enzyme complexes

# Time-resolved solution X-ray scattering of biomolecules

Sebastian Westenhoff<sup>1</sup>

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Photoactive enzymes modulate their activity according to light conditions. We have studied a series of photosensitive proteins, with the goal to identify their structural changes when they are photoswitched. I will present these results. The structural changes range from refolding and quaternary rearrangements in phytochromes, a coiled-coil transition in a light-gated histidine kinase, and redox-driven rearrangements in cryptochromes.

In order to obtain structural information in solution, we have used time-resolved solution X-ray scattering. I provide an overview over the technique and discuss how it can be used to provide specific information on structural changes in solution. In particular, I will present how model-free structural parameters can be extracted, and how more detailed structural models can be generated and validated against the difference scattering data.

A bottleneck of time-resolved X-ray scattering is the lack of structural specificity. This could be mitigated by fluctuation scattering approaches, which may become available at the European XFEL.

## References

- [1] O. Berntsson, R. P. Diensthuber, M. R. Panman, A. Björling, A. J. Hughes, L. Henry, S. Niebling, G. Newby, M. Liebi, A. Menzel, R. Henning, I. Kosheleva, A. Möglich, and S. Westenhoff, "Time-Resolved X-Ray Solution Scattering Reveals the Structural Photoactivation of a Light-Oxygen-Voltage Photoreceptor," **Structure**, vol. 25, no. 6, p. 933–938.e3, Jun. 2017.
- [2] O. Berntsson, R. P. Diensthuber, M. R. Panman, A. Björling, E. Gustavsson, M. Hoernke, A. J. Hughes, L. Henry, S. Niebling, H. Takala, J. A. Ihalainen, G. Newby, S. Kerruth, J. Heberle, M. Liebi, A. Menzel, R. Henning, I. Kosheleva, A. Möglich, and S. Westenhoff, "Sequential conformational transitions and  $\alpha$ -helical supercoiling regulate a sensor histidine kinase," **Nat. Comm.**, vol. 8, no. 1, p. 284, Aug. 2017.
- [3] A. Björling, O. Berntsson, H. Lehtivuori, H. Takala, A. J. Hughes, M. Panman, M. Hoernke, S. Niebling, L. Henry, R. Henning, I. Kosheleva, V. Chukharev, N. V. Tkachenko, A. Menzel, G. Newby, D. Khakhulin, M. Wulff, J. A. Ihalainen, and S. Westenhoff, "Structural photoactivation of a full-length bacterial phytochrome," **Sci. Adv.**, vol. 2, no. 8, p. e1600920, Aug. 2016.
- [4] A. Björling, S. Niebling, M. Marcellini, D. Van Der Spoel, and S. Westenhoff, "Deciphering solution scattering data with experimentally guided molecular dynamics simulations," **J. Chem. Theory Comput.**, vol. 11, no. 2, pp. 780–787, Jan. 2015.

**Structural dynamics of haemoproteins using  
synchrotron radiation  
and  
X-ray free electron lasers**

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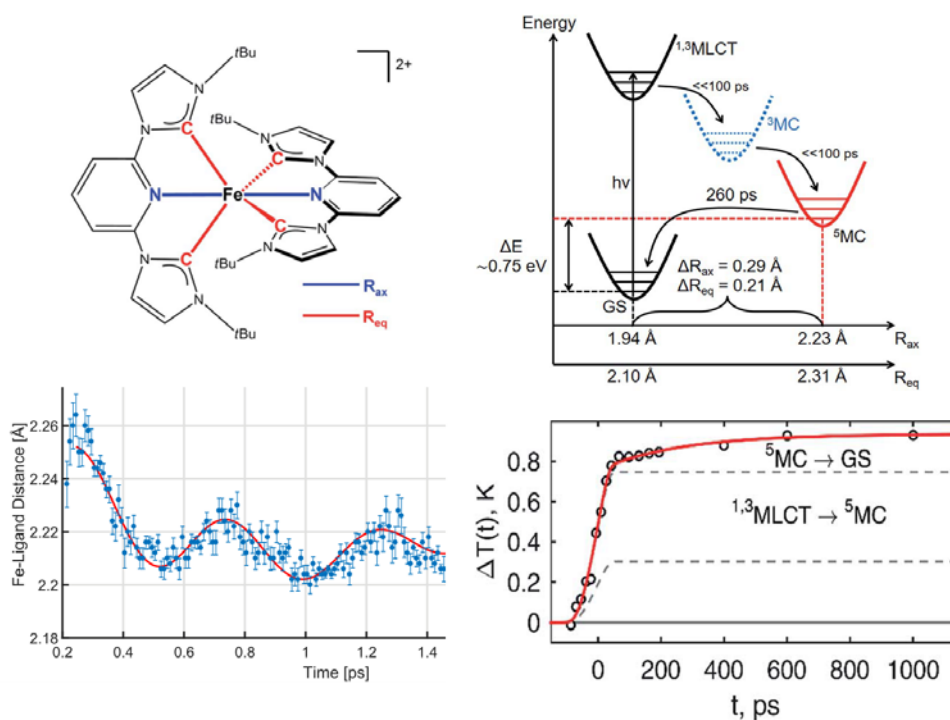
I will present X-ray spectroscopic studies at the Iron K-edge of myoglobin-NO and cytochrome c with 100 ps resolution at the Swiss Light Source (Silatani et al, PNAS 2015) and of myoglobin-NO and cytochrome c with 100 fs resolution at the Eu-XFEL (Hamburg), SACLA (Japan) and swissFEL (Villigen).

# Unpacking energetics and dynamics in photoexcited transition-metal complexes with synchrotrons and XFELs

Haldrup K.<sup>1</sup>, Nielsen M.M.<sup>1</sup> *et al.*

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This talk will describe a series of recent investigations of how the photon energy is redistributed on internal and external degrees of freedom following photo-excitation of transition-metal centered complexes [1-8]. Special emphasis will be on how combining and extending established X-ray methodologies at synchrotron and XFEL beamlines can yield new insights on both electronic and structural dynamics, as well as information on the interplay between solute and solvent.



**Figure 1:** Molecular structure, potential energy landscape, structural dynamics and solvent temperature change following photo-excitation of an Fe-centered compound.

## References

- [1] – K. Haldrup *et al.*, *Journal of Physical Chemistry A* (2012)
- [2] – G. Vanko *et al.*, *Journal of Electron Spectroscopy and Related Phenomena* (2013)
- [3] – S. Canton *et al.*, *Nature Communications* (2015)
- [4] – T. van Driel *et al.*, *Nature Communications* (2016)
- [5] – K. Haldrup *et al.*, *Journal of Physical Chemistry B* (2016)
- [6] – E. Biasin *et al.*, *Physical Review Letters* (2016)
- [7] – D. Leschev *et al.*, *Chemical Science* (2017)
- [8] – K. Kjær *et al.*, *Physical Chemistry Chemical Physics* (2018)

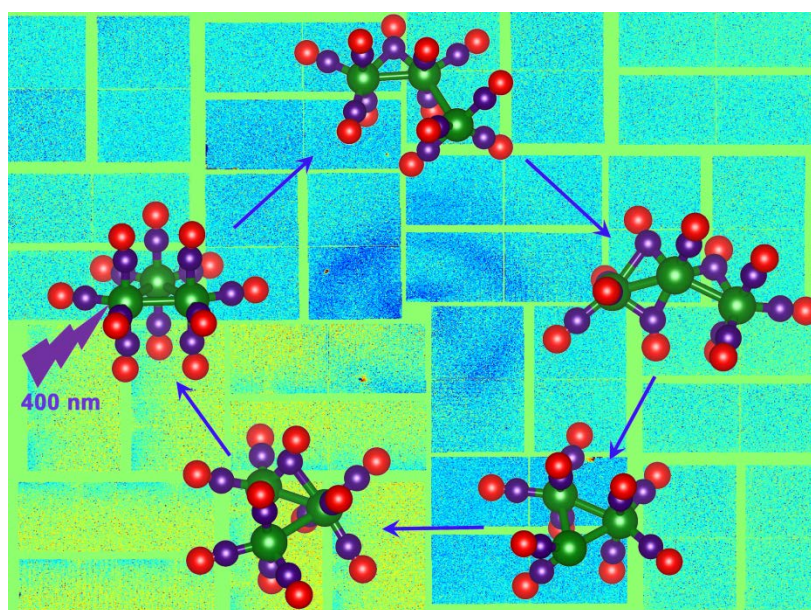
# Photochemical reaction dynamics of $\text{Ru}_3(\text{CO})_{12}$ studied by picosecond and femtosecond X-ray solution scattering at ESRF and LCLS

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A more complete mechanism for the photofragmentation of  $\text{Ru}_3(\text{CO})_{12}$ , a prototype for the photochemistry of transition metal carbonyls, following 400 nm excitation was obtained from a combination of ps and fs X-ray solution scattering at the synchrotron<sup>1</sup> and XFEL<sup>2</sup>. 400 nm laser excitation selectively breaks a single Ru-Ru bond to form  $\text{Ru}_3(\text{CO})_{11}(\mu\text{-CO})$ .  $\text{Ru}_3(\text{CO})_{11}(\mu\text{-CO})$  loses one CO forming  $\text{Ru}_3(\text{CO})_8(\mu\text{-CO})_3$  with a characteristic timescale of 1.5 ps, which in turn loses another CO and also reforms the Ru-Ru bond to yield  $\text{Ru}_3(\text{CO})_{10}$  on a time scale of 10 ps.  $\text{Ru}_3(\text{CO})_{10}$  dominates from 10 ps to 100 ns<sup>1</sup>, and rebinds one CO to form  $\text{Ru}_3(\text{CO})_{10}(\mu\text{-CO})$ <sup>1,3</sup>, which eventually relaxes to the starting molecule by binding another CO. These results indicate that contrary to long standing hypotheses, metal-metal bond breakage is the only chemical reaction immediately following the photolysis of  $\text{Ru}_3(\text{CO})_{12}$  at 400 nm.



## Photoreaction pathways of $\text{Ru}_3(\text{CO})_{12}$ in $\text{C}_6\text{H}_{12}$ following 400 nm excitation

### References

1. Q. Y. Kong, *et al. Angew. Chem. Int. Ed.* 47, 5550 (2008).
2. Q. Y. Kong, *et al. Photochem. Photobiol. Sci.* DOI: 10.1039/c8pp00420j
3. E. A. Glascoe, *et al. Organometallics*, 25, 775 (2006).

# **FXE instrument of the European XFEL: experimental capabilities and first results**

Khakhulin D.<sup>1</sup>, Alves Lima F.<sup>1</sup>, M. Biednov M.<sup>1</sup>, Galler A.<sup>1</sup>,  
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Recent development of optical pump/X-ray probe techniques at large scale facilities such as synchrotrons and X-ray free-electron laser (XFEL) sources enabled direct visualization of various fundamental ultrafast phenomena in solution photochemistry and photophysics of solids. Due to intrinsically much shorter pulses, the temporal resolution of such experiments at XFELs is over three orders of magnitude higher compared to that at conventional synchrotron sources, reaching the sub-100 fs domain. On the other hand, great stability of the X-ray radiation, flexibility of standard setups and relatively good availability of beamtime for users makes synchrotron sources indispensable for establishing new experimental methodologies and performing extended systematic investigations of transient processes specifically on the timescales spanning the range from a hundred of picoseconds to milliseconds. Taking advantage of complementary synchrotron and XFELs experiments and combining structurally and electronically sensitive probes, namely time-resolved X-ray scattering/diffraction [1], X-ray emission [2] and absorption [3] spectroscopies in one study [4,5], it has become possible to accurately monitor intrinsically coupled electronic and structural transformations in photo-responsive materials and solvated molecular systems throughout the complete excitation/relaxation cycle.

The design of the Femtosecond X-ray Experiments (FXE) instrument of the European XFEL, which came online only about 1.5 years ago, was to a large extent inspired by the synchrotron-developed methodologies of combining simultaneous structural and electronic observables at kHz and MHz repetition rates. In this contribution we will present the progress of the FXE instrument commissioning over the past year, describe current capabilities of the setup as well as the first experimental results. Particularly, the important role of synchrotron experiments in understanding various ultrafast laser-driven phenomena will be demonstrated and emphasized.

## **References**

- [1] H. Ihee et al., *Science*, 309, 5738 (2005)
- [2] G. Vankó et al., *Angew. Chem.*, 122, 6046 (2010)
- [3] Ch. Bressler et al., *Science*, 323, 489 (2009)
- [4] Ch. Bressler et al., *Faraday Discuss.*, 171, 169 (2014)
- [5] S.E. Canton et al., *Nat. Comm.*, 6, 6359 (2015)

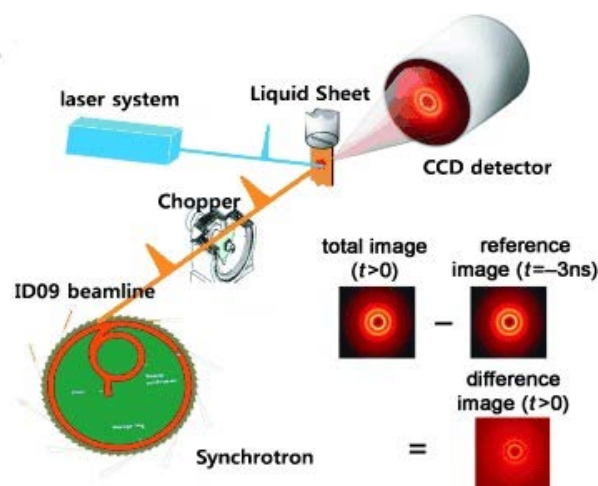
# Time-resolved structural studies at the ID09 beamline of the ESRF

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The ID09 beamline of the ESRF is the most advanced synchrotron beamline for time-resolved structural studies in Europe. The availability of an intense pink beam, single X-ray pulse selection and the flexibility of its sample environment with different kind of laser excitation options are the key characteristics of the beamline. Experiments currently performed at ID09 range from ultrafast dynamics studies in solid state systems [1] to slow (up to hundreds of milliseconds) conformational changes in large biological molecules [2]. I will describe the current status of the beamline and present examples of recent research that highlight the complementarity between ID09 and pump-probe beamlines at X-ray free-electron lasers.



**Figure 1:** Schematic of ID09 setup for time-resolved X-ray scattering experiments on chemical reactions in solution (adapted from [3]).

## References

- [1] - M. Sander, M. Herzog, J. E. Pudell, M. Bargheer, N. Weinkauff, M. Pedersen, G. Newby, J. Sellmann, J. Schwarzkopf, V. Besse, V. V. Temnov, and P. Gaal, *Phys. Rev. Lett.* **119**, 075901, (2017).
- [2] - I. Josts, S. Niebling, Y. Gao, M. Levantino, H. Tidow and D. Monteiro, *IUCrJ* **5**, 667-672, (2018).
- [3] - T. K. Kim, J. H. Lee, M. Wulff, Q. Kong, H. Ihee, *ChemPhysChem* **10**, 1958-1980, (2009).

# Time-resolved nanoscience – Between molecular kinetics and solid-state dynamics

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Nanoscale excitation of mesoscale objects often displays unexpected dynamics and structural relaxations, which can be harnessed in photonic applications [1,2]. A more complete understanding may require both the ultrashort time scales [3] accessible at FEL sources as well as detailed mapping of excitation scales [4,5] on modern ring sources [7]. Often different length scales are involved, in particular in hybrid materials [8]. In this talk the different questions will be classified in terms of the path to address them by the respective experimental approaches.

## References

- [1] A. Plech, V. Kotaidis, S. Grésillon, C. Dahmen and G. von Plessen: *Laser-Induced heating and melting of gold nanoparticles studied by time-resolved x-ray scattering*, Phys. Rev. B 70 (2004) 195423.
- [2] V. Kotaidis and A. Plech: *Cavitation dynamics on the nanoscale*, Appl. Phys. Lett. 87, (2005) 213102.
- [3] A. Plech, V. Kotaidis, M. Lorenc, J. Boneberg: *Femtosecond laser near-field ablation from gold nanoparticles*, Nature Phys. 2 (2006) 44; A. Plech, P. Leiderer, J. Boneberg: *Femtosecond near field ablation*, Laser & Phot. Rev. 3 (2009) 435.
- [4] V. Kotaidis, C. Dahmen, G. von Plessen, F. Springer, A. Plech: *Excitation of nanoscale vapor bubbles at the surface of gold nanoparticles in water*, J. Chem. Phys., 124 (2006) 184702.
- [5] A. Siems, S. Weber, J. Boneberg and A. Plech: *Thermodynamics of nanosecond nanobubble formation at laser-excited metal nanoparticles*, New. J. Phys. 13 (2011) 043018.
- [6] A. Plech, S. Ibrahimkuty, S. Reich, G. Newby: *Thermal dynamics of pulsed-laser excited gold nanorods in suspension*, Nanoscale, 9 (2017) 17284-17292; A. Plech, S. Ibrahimkuty, D. Issenmann, V. Kotaidis, A. Siems, *Ultrafast x-ray scattering on nanoparticle dynamics*, J. Phys.:Conf. Ser. 425 (2013) 092008.
- [7] A. Plech, V. Kotaidis, K. Istomin, M. Wulff: *Small angle pump-probe studies of photo-excited nanoparticles*, J. Synchr. Rad., 14 (2007) 288.
- [8] S. Ibrahimkuty, J. Kim, M. Cammarata, F. Ewald, J. Choi, H. Ihee, A. Plech: *Ultrafast structural analysis of photo-excited protein hybrid nanoparticles*, ACS Nano 5 (2011) 3788.



# Time-resolved synchrotron XRD of shock compressed matter: the case study of Bi

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The group V metal bismuth (Bi) is well-known for exhibiting a large number of polymorphic transitions within a low pressure and temperature region [1]. Within 3 GPa (1 GPa = 10000 bar), it undergoes the I-II and the II-III transitions and the III-V transition above 7 GPa. At high temperature, between 2.5 and 6 GPa, phase II transforms into Bi-IV. This view of the Bi-phase diagram can be drastically altered by metastable effects in static compression experiments [2], with the appearance of phase V at pressures as low as 5 GPa for example. Moreover it was recently shown in a static study that hydrostaticity conditions have an important effect on the melting line of bismuth, which in turn is found to be much higher.

Synchrotron ns time-resolved X-Ray Diffraction has been performed on this complex system under dynamical load along various compression and release paths, hence exploring the Bi phase diagram up to 8 GPa and 600 K. Marked departures from the equilibrium behaviour are observed. The sequence of structural changes is different upon compression and release. Bi-III, the complex host-guest structure is never observed. Instead Bi-V is observed over a large domain. Melting of Bi-V and crystallization of the fluid into Bi-I are clearly identified on stress release. These observations on a prototypical system underline the possible difficulties of disclosing equilibrium structural transformations at high pressure by using dynamic compression and highlight the need of XRD for such studies.

After presenting our results on Bi, we will discuss about the complementarities between the synchrotron and the XFEL for the study of matter under dynamic compression. Finally some perspectives for the ESRF upgrade will be given.

## References

- [1] – E. Yu and E. G. Ponyatovsky, CRC Press
- [2] – E. Principi et al., Phys. Rev. B 74, 064101 (2006)
- [3] – C. Lin et al., Nature Comm. 8, 14260 (2017)

# Studying Complex Chemical Reactions at Pulsed High-flux X-ray Sources

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Common for time-resolved X-ray experiments is the applied pump / probe scheme, often with an optical pump-laser initiating a chemical reaction whose structural time evolution is then investigated by X-ray probe pulses at various time delays (picoseconds for synchrotron X-ray sources, and femtosecond for X-ray Free Electron Lasers). X-ray photon-in / photon-out techniques are based on X-ray diffraction, X-ray scattering or x-ray spectroscopic techniques like near edge spectroscopy or X-ray emission spectroscopy. Meanwhile X-ray spectroscopic techniques probe the local environment around specific atoms in a molecule - such as orbitals, X-ray diffraction and x-ray scattering studies reveal the structure of the bulk of periodic or disordered systems.

Two detailed examples of very recent synchrotron and FEL research will be given, where ultrafast optical spectroscopy and highly brilliant, ultrafast X-ray-pulse-based structural dynamics methods have been developed as complementary tools for studying the real time structure-function relationships in (i) complex chemical reactions and of (ii) bio-mimicking opto-electronic devices and energy materials. The findings will be discussed in the context of novel analysis approaches overcoming the classical description of uni- and bimolecular reactions in the traditional framework of chemistry.

## References

- [1] - S. Bari, R. Boll, K. Idzik, K. Kubiček, D. Raiser, S. Thekku Veedu, Z. Yin, S. Techert, *Ultrafast Time Structure Imprints in Complex Chemical and Biochemical Reactions*, chapter 15, eds. U. Bergmann, V. Yachandra, J. Yano, *Fundamentals and Application of Free Electron Lasers*, Royal Chemical Society, Oxford, 301-322, (2017). doi: 10.1039/9781782624097 and references therein.
- [2] - S. Thekku Veedu, S. Bari, S. Techert, *Development of Ultrafast X-ray Free Electron Laser Tools in (Bio)Chemical Research*, Springer Science, Berlin, in press (2019).

# Complementarity of SR and XFEL sources for tracking chemical reactions in solution with ultrashort X-ray pulses

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Complemental use of synchrotron radiation (SR) and X-ray free electron laser (XFEL) sources is now essential for successful time-resolved X-ray studies. Here I show examples of tracking chemical reactions in solution by combined use of PF-AR (KEK) and SACLA (RIKEN/SPring-8).

Bond formation is an essential process in chemistry, but it is challenging to keep track of detailed atomic movements associated with bond formation because of its bimolecular nature. Bond formation in solution phase has been especially elusive because it is difficult to initiate and follow such diffusion-limited bimolecular processes with ultrafast time resolution. In this regard, Au oligomer complex,  $[\text{Au}(\text{CN})_2^-]_n$ , offers a good model system in which to study the dynamics of bond formation in solution [1,2]. Using femtosecond time-resolved X-ray scattering, we successfully visualized in real time the birth of a gold trimer complex,  $[\text{Au}(\text{CN})_2^-]_3$ , that occurs via photo-induced formation of Au-Au covalent bonds [3].

The ground state of the trimer has Au atoms that are weakly bound to each other by aurophilic interaction and aligned in a bent geometry. Upon photoexcitation, the ground state rapidly converts into the first excited state where Au-Au covalent bonds are formed among Au atoms aligned in a linear geometry. Subsequently, the state transforms to a triplet state in 1.6 ps while accompanying further contraction of Au-Au bonds by 0.1 Å (studied at SACLA). Later, the triplet state of the trimer converts to a tetramer on nanosecond time scale (studied at PF-AR). This work showcases the possibility of tracking detailed structural changes in solution with sub-ps temporal and sub-angstrom spatial resolutions, thanks to the combined use of SR and XFEL.

## References:

- [1] Rawashdeh-Omary, M. A., Omary, M. A., Patterson, H. H. & Fackler, J. P., *J. Am. Chem. Soc.* 123, 11237–11247 (2001).
- [2] Iwamura, M., Nozaki, K., Takeuchi, S. & Tahara, T., *J. Am. Chem. Soc.* 135, 538–541 (2013).
- [3] Kim, K. H., Kim, J. G., Nozawa, S., Sato, T., Oang, K. Y., Kim, T. W., Ki, H., Jo, J., Park, S., Song, C., Sato, T., Ogawa, K., Togashi, T., Tono, K., Yabashi, M., Ishikawa, T., Kim, J., Ryoo, R., Kim, J., Ihee, H. & Adachi, S., *Nature*, 518, 385-389 (2015).

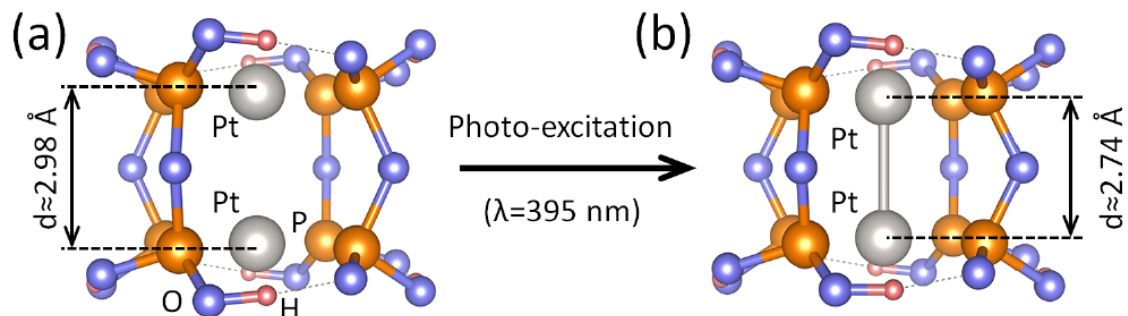
# Kinetics and dynamics in bi-metallic complexes in solutions

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Metal complexes, and not least the d8 systems, are important model systems for catalysis and energy applications as well as fascinating playgrounds for testing new methods for predicting and measuring structural dynamics and what goes on in the interface between molecules and their surroundings.

I will draw a few lines from our work at synchrotron sources to recent hard X-ray pump-probe experiments conducted at XFELs, using X-ray scattering to measure the structural response of solvated metal complexes to optical excitation. Coupling these experiments with model calculations, we were able to track the coupling between structural change of the solute and reorganization of solvent molecules, the formation and decay of excited state complexes, and even to track the ground state dynamics using off resonance excitation [1]. The data quality could be enhanced by exploiting the anisotropy induced by selectively exciting a subset of solute molecules with specific orientations of their transition dipole moments [2].



**Figure 1:** (a) Structure of the PtPOP ( $[\text{Pt}_2(\text{P}_2\text{O}_5\text{H}_2)_4]^{4+}$ ) metal complex in the ground state. (b) Structure of PtPOP molecule in the excited state. The formation of bond between the two Pt atoms leads to a contraction of about  $0.24 \text{ \AA}$ .

## References

[1] Haldrup, K., Levi, G., Biasin, E., Vester, P., Laursen, M. G., Beyer, F., ... Nielsen, M. M. (2019). Ultrafast X-Ray Scattering Measurements of Coherent Structural Dynamics on the Ground-State Potential Energy Surface of a Diplatinum Molecule. *Physical Review Letters*, 122(6), 063001. <https://doi.org/10.1103/PhysRevLett.122.063001>

[2] Biasin, E., van Driel, T. B., Levi, G., Laursen, M. G., Dohn, A. O., Moltke, A., ... Nielsen, M. M. (2018). Anisotropy enhanced X-ray scattering from solvated transition metal complexes. *Journal of Synchrotron Radiation*, 25(2), 306–315. <https://doi.org/10.1107/S1600577517016964>

# **Implementation of a high repetition and short pulse option at ID09**

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I will discuss a beamline upgrade proposal that aims for realizing optical pump - x-ray probe experiments at repetition rates of up to 50 kHz. The upgrade exploits the improved beam properties of the new ESRF-EBS storage ring and increases the photon flux by two orders of magnitude. A key component is the installation of a new femtosecond high-frequency laser source. In addition, the proposal involves implementation of a short (i.e., sub 10 ps) x-ray pulse option by introducing a photoacoustic Bragg switch. After introducing specifications of the upgrade proposal I will also discuss exemplary scientific cases for future time-resolved experiments at ID09.

# Chemical information in X-ray emission spectroscopy

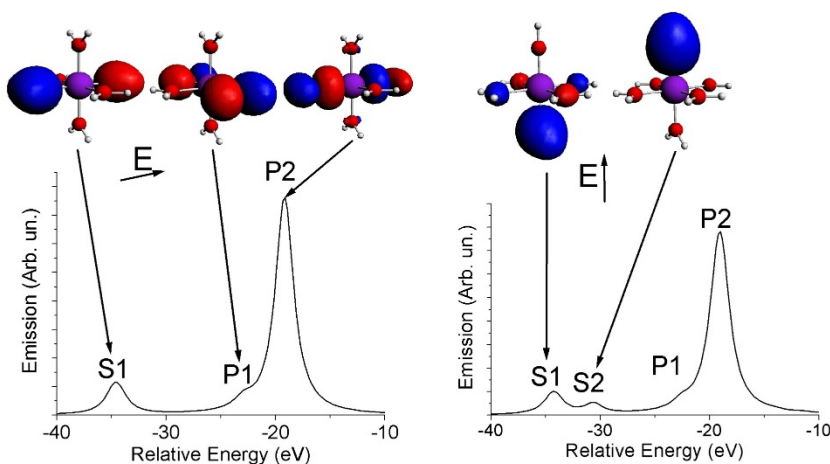
Pieter Glatzel

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X-ray emission spectroscopy is a second order process following core shell ionization. The technique does not require a monochromatic incident X-ray beam and is thus attractive for applications at free electron lasers and pink beam synchrotron radiation beamlines. The past decades have brought significant new insight into the theoretical understanding of X-ray emission spectra which in turn considerably increased the value of the technique for time-resolved experiments.

The strong  $K\alpha$  and  $K\beta$  emission lines have been used with great success to characterize the spin state of a 3d transition metal ion. The much weaker valence-to-core lines give direct access to the valence electron configuration and thus contain a wealth of chemical information. However, obtaining sufficient data quality for a detailed analysis is challenging and pump-and-probe experiments.

The presentation will discuss some fundamental aspect of X-ray emission spectroscopy and address experimental challenges.



## References

- [1] – P. Glatzel and U. Bergmann, *Coord. Chem. Rev.* **249**, 65-95 (2005)
- [2] – E. Gallo and P. Glatzel, *Advanced Materials*, **26**, 7730-7747 (2014)

## Excited state of Cu-based OLED material is probed with pump-probe XAS, XES and WAXS

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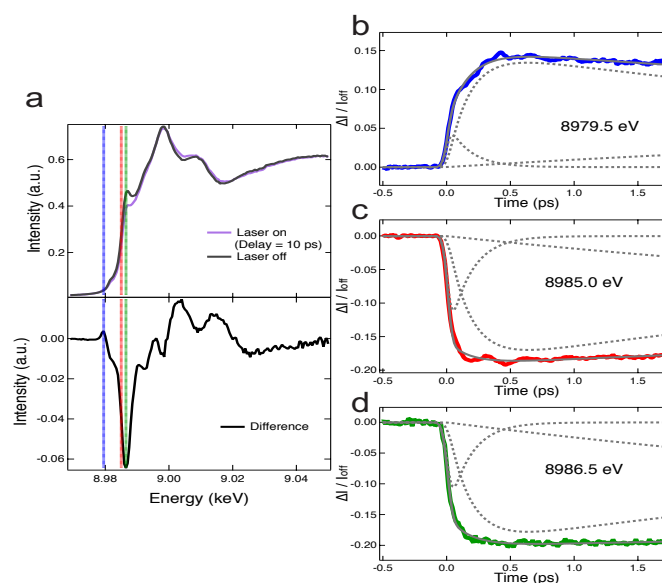
Organic Light Emitting Diodes (OLEDs) depict an economical and efficient technology for e.g. flexible displays and innovative area lighting. The main challenge in this regard is to develop efficient emitting materials, which do not contain rare transition metal ions as this has a significant impact on the cost-efficient production of OLED devices. We recently proposed a new multinuclear Cu complex as a new promising compound for such applications. For rational development of efficient OLED materials and understanding of non-radiative losses, experimental data about structural changes and charge movements between atoms of the complex in the excited state are needed. In particular, the following questions have to be addressed: i) are phosphorus-coordinated or carbon-coordinated Cu atoms are involved in the charge transfer ii) how the structure, in particular, Cu-Cu distances change in the excited state iii) are phosphorus atoms involved in the charge transfer forming the excited state. I will show how we used the combination of pump-probe WAXS (ID09, ESRF), pump-sequential-probes XAS (SuperXAS, SLS) and pump-probe XES at P K-alpha line (Alvra, SwissFEL) to address these questions. Preliminary data on Cu K-beta XES and WAXS from the experiment at FXE of European XFEL will be also discussed. We will demonstrate how complementarity of pump-probe experiments at all these facilities allows to understand the excited states of the complex.

# Time-resolved X-ray Spectroscopy: From the nano to the femtosecond regimes

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Advances in experimental methodology aligned with technological developments, such as X-ray Free Electron Lasers (X-FELs) and High Harmonic Generation (HHG), has led to a paradigm shift in the capability of X-ray Spectroscopy to deliver simultaneously high temporal and spectral resolution. However, given the availability of X-FELs, 3<sup>rd</sup> generation light sources, which have a temporal resolution limited to the picosecond regime, remain the work horses of time-resolved structural dynamics.



Importantly, the complex nature and high information content of this class of techniques means that detailed theoretical studies are often essential to provide a firm link between the spectroscopic observables and the underlying molecular structure and dynamics. For X-FELs, the understanding the femtosecond dynamics of molecules in electronically excited states requires simulations that go beyond the single nuclear configuration regime and the Born-Oppenheimer approximation.

Herein I will present some recent work on simulating and understanding ultrafast X-ray spectra using excited state simulations based upon quantum nuclear dynamics. This will include prediction and experimental realisation of ultrafast time-resolved experimental signals of a Cu transition metal complex (Figure 1) and new avenues, which exploit on-the-fly quantum dynamics simulations to reduce the computational expense of these calculations. I will also present potential experiments and opportunities to shed insight into dynamics which other techniques cannot achieve.

1. T. J. Penfold, E. Gindensperger, C. Daniel and C. M. Marian, *Chem. Rev.*, **118**:6975 (2018).
2. G. Capano, C.J. Milne M. Chergui, U. Rothlisberger, I. Tavernelli and T.J. Penfold *J. Phys. B* **48**:214001 (2015).



# **Multiscale dynamics studied with Xrays: from molecular switching to material transformation**

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The general excitement born out of ability to access the ultrafast time scales has caused rush of new ideas, new materials, and new instruments. One feat in particular has been draining a lot of effort, namely the control of materials with an ultrashort laser pulse. There is ample evidence now that materials can be directed between different macroscopic states by using appropriate electronic, or structural, excitations. The switching with a laser pulse of such materials can severely change their macroscopic properties (electric conductivity, magnetism, colour, etc.), whereby emerging cooperativity and coherence of different degrees of freedom underpin the resulting phase transitions of various sorts. However, the pertinent time scales for photo-switching processes in materials have been rather difficult to scrutinise. The pioneering investigations dealt mainly with the electron/phonon dynamics immediately following the femtosecond excitation, or the kinetics of recovery to the thermally stable states. This situation is changing fast today. Time-resolved X-ray diffraction and ultrafast VIS-IR spectroscopy reveal that the degrees of freedom triggered by a femtosecond laser pulse in a material follow a sequence in the out-of-equilibrium dynamics. Those steps dissected in time, provided a mechanistic picture of a material transformation driven under different, non-thermal and thermal, regimes.

# **Experiences from the LCLS**

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X-ray free electron lasers have made the sub-ps timescales accessible for X-ray pump/laser probe experiments. Here I will present some of the experiences from the XPP and XCS beamlines at LCLS as well as some of the strengths, weaknesses and challenges that we face now and going forward. As FEL techniques and facilities mature, there are still a number of challenges to address and areas where synchrotron and FEL experiments differ. In order to exploit the synergies of Synchrotron and XFEL experiments, some of these differences need to be highlighted, detailed and characterized, such that robust scientific conclusions can be more easily reached by the user community in general.

# Charge-density waves at the femto- and picosecond time scales

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Spin- (SDW) and Charge-density wave (CDW) states are ubiquitous in solid state physics. They both correspond to a modulation of the spin or the charge density with twice the Fermi wave vector of the electron gas. As both states are gapped, they are sensitive to impulsive absorption of laser infrared pulses, which induces phase transformations. Interestingly enough, CDW are generally coupled to the lattice, which gives rise to satellite reflections easy to observe by X-ray diffraction.

In this work, we compare the dynamical behavior of CDW after an infrared laser pulse in three different DW systems: Chromium [1],  $K_{0.3}MoO_3$  (so-called blue bronze) [2], and 1T-TaS<sub>2</sub> [3,4]. We used pump-probe diffraction techniques to follow the incommensurate satellite reflections (position, width and intensity) as a function of the delay between the infrared pulse and the X-ray pulse. At the femtosecond time scale (100 fs), the CDW amplitude is strongly depressed after the pulse, which leads to the melting of the CDW state in a few ps [1,2]. This melting is driven by a coherent phonon mode corresponding to the CDW amplitude mode. At the picosecond (100 ps) timescale, other phenomena are observed depending on the sample. In the 1T-TaS<sub>2</sub> case, another CDW phase is photo-induced and develops by a fast sub-ns nucleation-growth-coarsening process never observed before [3,4]. At longer delays, the recovery of the initial CDW state follows different mechanisms which depend on the compound. In Chromium, a strange change in the satellite position suggests a physics governed by CDW dislocation gliding or climbing. All these examples show that CDW materials need to be studied at all time scales, ranging from fs, at XFEL, to ns, possibly at synchrotrons.

## References

- [1] - V.L.R. Jacques, C. Lauhé, N. Moisan, S. Ravy, and D. Le Bolloc'h, Phys. Rev. Lett. **117**, 156401 (2016).
- [2] - T. Huber, S.O. Mariager, A. Ferrer, H. Schäfer, J.A. Johnson, S. Grübel, A. Lübke, L. Huber, T. Kubacka, C. Dornes, C. Lauhé, S. Ravy, G. Ingold, P. Beaud, J. Demsar, and S.L. Johnson, Phys. Rev. Lett. **113**, 156401 (2014).
- [3] - C. Lauhé, T. Huber, G. Lantz, A. Ferrer, S.O. Mariager, S. Grübel, J. Rittman, J.A. Johnson, V. Esposito, A. Lübcke, L. Huber, M. Kubli, M. Savoini, V.L.R. Jacques, L. Cario, B. Corraze, E. Janod, G. Ingold, P. Beaud, S. Johnson, and S. Ravy, Phys. Rev. Lett. **118**, (2017), 247401 (2017).
- [4] - G. Lantz, C. Lauhé, S. Ravy, M. Kubli, M. Savoini, K. Tasca, E. Abreu, V. Esposito, M. Porer, A. Ciavardini, L. Cario, J. Rittmann, P. Beaud, S. Johnson, Phys. Rev. **B 96**, 224101 (2017).

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