# MA 30: PhD Focus Session: Non-equilibrium dynamics in theory and experiment

Non-equilibrium phenomena often occur at the edge of phase transitions, for example, in maintaining the organism and cells, photosynthesis, or other exciting reactions. Nevertheless, many of these phenomena are poorly understood or require various disciplines to come together to understand these phenomena in a significant context. Here, however, there is still a need for communication between theory and experiment. Since today's experiments and ideas often have a large gap, we want to use this focus session to create an environment where young researchers can get an overall picture. In doing so, this Ph.D. focus session should emphasize highlights and show the current front of research, in addition to the character of tutorial lectures, and give a chance to conclude in a lively discussion. This PhD Focus Session is organized by Lea Spieker and Gérald Kämmerer (Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Germany).

Time: Wednesday 15:00–18:00 Location: HSZ 02

**Invited Talk** MA 30.1 Wed 15:00 HSZ 02

**Femto- phono- magnetism** — •Sangeeta Sharma — Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Max-Born-Str. 2A, 12489 Berlin, Germany

From the outset of research into femtomagnetism, the field in which spins are manipulated by light on femtosecond or faster time scales, several questions have arisen and remain highly debated: How does the light interact with spin moments? How is the angular momentum conserved between the nuclei, spin, and angular momentum during this interaction? What causes the ultrafast optical switching of magnetic structures? What is the ultimate time limit on the speed of spin manipulation? What is the impact of nuclear dynamics on the light-spin interaction?

In my talk I will advocate a parameter free ab-initio approach to treating ultrafast light-matter interactions, and discuss how this approach has led both to new answers to these old questions but also to the uncovering of novel and hitherto unsuspected early time spin dynamics phenomena. In particular I will show that selective excitation of phonon modes exert a strong influence on femtosecond demagnetisation. Our finding demonstrates that the nuclear system, typically assumed to play a role of an energy sink aiding remagnetization of the spin system, plays a profound role in controlling femtosecond demagnetization of magnetic materials.

**Invited Talk** MA 30.2 Wed 15:30 HSZ 02

**Spin-switchable molecules in interaction with their environment.** — •Cyrille Barreteau — University Paris-Saclay, CEA, CNRS,SPEC, 91191, Gif-sur-Yvette, France

Molecules that can switch spin-state form a very important class of molecules that offers a formidable test bed for fundamental studies and applied research due to the multiple possible channels to tune their properties. Spin-crossover (SCO) molecules are the most common spin-switchable molecules where the spin-state of the metal complex changes under the application of an external stimulus such as light, temperature, pressure etc.. SCO crystals have been the subject of intense studies however; it is much more recent that these molecules have been deposited on surfaces. In practice, the number of SCO that are robust enough to remain intact on surface and retain their switchability is rather limited. In addition, from the modelling point, these systems are also delicate to describe accurately. In this talk, I will present coupled experimental and theoretical results of various spin-switchable molecules that have successfully been deposited on inorganic surfaces. It will be shown how their properties are affected by their environment, in particular we will investigate the role of molecule-molecule and molecule-substrate interaction or the application of an electric field. This will provide us with the tools to manipulate the properties of such systems and give hint for possible strategies to optimize the magneto-transport properties of materials/devices.

**15 min. break**

**Invited Talk** MA 30.3 Wed 16:15 HSZ 02

**Yep, real photodoping.** — Lukas Gierster[1,2] and •Julia Stähler[1,2] — [1]Humboldt-Universität zu Berlin, Inst. f. Chemie, Berlin, Germany — [2]Fritz-Haber-Institut der MPG, Abt. PChem, Berlin, Germany

The advent of photoinduced phase transitions and the investigation of their non-equilibrium dynamics on ultrafast timescales coined various fashionable terms like *hidden phases*, *new phases of matter*, or *photodoping*. They were not always used rigorously and partially developed a life on their own. For instance, a photoexcited solid is not necessarily in a different phase just because it shows different properties than in its ground state - and the pure redistribution of charges after photoexcitation is not equivalent with chemical doping even if the photoexcitation drives a phase transition.

I will discuss these subtle, but important differences using the example of ZnO that undergoes a semiconductor-to-metal transition upon real photodoping at very low excitation densities [1]. Notably, the hidden, metallic phase has no equivalent in the equilibrium phase diagram and shows decay dynamics on ultrafast timescales, but can also be retained and become metastable [2].

[1] Nat. Commun. 12 978 (2021)
[2] Faraday Disc. (2022) DOI:10.1039/D2FD00036A

**Invited Talk** MA 30.4 Wed 16:45 HSZ 02

**Probing ultrafast magnetization thanks to ultrashort soft X-ray pulses** — •Emmanuelle Jal — Sorbonne Université, CNRS, Laboratoire de Chimie Physique - Matière et Rayonnement, LCPMR, Paris 75005, France

Even after more than 25 years of studies and debates, the mechanisms of ultrafast demagnetization remain disputed. In order to bring new experimental information into this field, and with the advent of femtosecond X-rays sources, new time-resolved XUV and soft X-ray-based pump/probe techniques are performed on magnetic thin films. During this talk, I will give an overview of what can be done with XUV and soft x-ray short pulses to probe electronic, magnetic, and structural dynamics. A special emphasis will be given to (i) simultaneous electronic and magnetism dynamics [1,2] and (ii) simultaneous structural and magnetism dynamics [3, 4,5].

[1] Rösner et al. Struct. Dyn. 7, 054302 (2020)
https://doi.org/10.1063/4.0000033
[2] Hennes et al Appl. Sci. 11m 325 (2021)
https://doi.org/10.3390/app11010325
[3] Jal et al. Phys. Rev. B 95, 184422 (2017)
https://doi.org/10.1103/PhysRevB.95.184422
[4] Chardonnet et al. Struct. Dyn. 8, 034305 (2021)
https://doi.org/10.1063/4.0000109
[5] V. Chardonnet, PhD 2022
https://tel.archives-ouvertes.fr/tel-03864973

**45 min. Panel discussion with all speakers**