TUT 1: Tutorial: Ferroics and Skyrmions

This tutorial combines the field of ferroics and domain engineering, their key concepts and materials with recent developments in strongly correlated systems, mainly focusing on skyrmions with polar textures. The basic concepts are introduced which intend to help non-specialists to get informed and involved in these interesting topics. This tutorial launches a 4-day focus (Plenary, Symposium, Focus Sessions and Posters) on ferroics, domain walls, multiferroics and skyrmion systems aiming at inspiring topical discussions to stimulate a vivid scientific exchange.

Organizers: Stephan Krohns, Dennis Meier, Elisabeth Soergel

Time: Sunday 16:00–18:30 Location: HSZ 304

Tutorial TUT 1.1 Sun 16:00 HSZ 304
Introduction to ferroic materials — •Claude Ederer — Materials Theory, ETH Zürich, Switzerland

In this tutorial talk I will give a general introduction to the physics of ferroic materials. I will discuss different cases such as ferro- and antiferromagnets, ferroelectrics, ferroelastics, and multiferroics. The basic phenomenology of ferroics will be introduced on the level of Landau theory, which allows to distinguish proper and improper ferroics and also to describe possible coupling between different ferroic order parameters. The important role of symmetry will be highlighted and microscopic mechanisms that drive the formation of ferroic orders will be mentioned.

Tutorial TUT 1.2 Sun 16:50 HSZ 304
Skyrmions with ferroelectric polarization in multiferroic lacunar spinels — •Alois Loidl — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

This tutorial will provide an introductory discussion of polar properties induced by topological spin order. Lacunar spinels will be taken as illuminating examples. They undergo orbital ordering and at low temperatures reveal complex magnetic phases. GaV_4S_8 and GaV_4Se_8 show ferromagnetic, cycloidal and Néel-type skyrmion lattice phases [1,2]. We provide a thorough study of the polar properties and show that the orbitally ordered phases are ferroelectric [3]. Moreover, spin-driven excess polarizations emerge in all magnetic phases. Hence, they host a zoo of multiferroic phases including the skyrmion lattice of spin vortices dressed with ferroelectric polarization [3]. The low-temperature magnetic phase diagrams document the importance of anisotropy: GaV_4S_8 is an easy axis magnet with a narrow skyrmion-lattice pocket only. In clear distinction, GaV_4Se_8 is governed by easy plane anisotropy, its skyrmion phase is drastically extended and reaches from the magnetic phase boundary down to the lowest temperatures.

[1] I. Kézsmárki *et al.*, Nature Materials **14**, 1116 (2015).
[2] S. Widmann *et al.*, Phil. Mag. (2016), in press.
[3] E. Ruff *et al.*, Science Advances **1**, E1500916 (2015).

Tutorial TUT 1.3 Sun 17:40 HSZ 304
Skyrmions in magnetic materials — •Jonathan White — Paul Scherrer Institut, Switzerland

Research into magnetic Skyrmions currently attracts significant attention in topological condensed matter physics. Individual Skyrmions display a non-trivial twisted spin structure which, unlike simple ferromagnetic and antiferromagnetic spin structures, is described in terms of a finite topological index. We will introduce how this finite topology endows Skyrmions with remarkable properties, which moreover display a novel interplay with the general properties and dimensionality of the host magnet. We will also explain how the fascinating aspects of the physics of Skyrmions motivates the general expectation that topological spin structures will become pivotal components for future information technology and data storage.

TUT 2: Tutorial: Micromagnetic Simulations

Organizers: Karin Everschor, Pedram Bassirian (Johannes Gutenberg Universität Mainz)

In the field of spintronics, micromagnetic simulations are an essential tool to predict new and explain existing phenomena. Nowadays various micromagnetic simulation softwares based on different solving techniques are available and they have accelerated research in different fields of spintronics. The goal of this tutorial is to provide a broad overview of different codes available and of what they are capable of doing. In particular it should be highlighted where the different simulators are good at. With this tutorial we aim to improve the general understanding and applicability of micromagnetic simulations and encourage people to use them more frequently and accurately in their research.

Time: Sunday 16:00–18:30 Location: HSZ 401

Tutorial TUT 2.1 Sun 16:00 HSZ 401
An overview of mumax3 with a spotlight on its newest features — Arne Vansteenkiste[1], •Jonathan Leliaert[1], Mykola Dvornik[2], Mathias Helsen[1], Felipe Garcia-Sanchez[3], and Bartel Van Waeyenberge[1] — [1]Ghent University, Ghent, Belgium — [2]University of Gothenburg, Gothenburg, Sweden — [3]INRIM, Turin, Italy

In this talk an overview is given of the GPU-accelerated micromagnetic software package MuMax3, developed at the DyNaMat group at Ghent University. This software solves the time- and space dependent evolution of the magnetization on the nano- to micro scale using a finite-difference discretization. Its high performance and low memory requirements allow for large-scale simulations to be performed in limited time and on inexpensive hardware. We begin with a short introduction to micromagnetism. Next, with the help of live demos, it is shown how to use this software either in its user-friendly web-interface, or via input-files for more complex simulations. Finally, we introduce three new features: first, mumax3-server allows to share simulations between different computers to efficiently execute large batches of simulations. Second, the adaptive time-step algorithm was extended to also simulate nonzero temperatures with optimal performance. Third, we present the possibility to include custom energy terms increases the users* freedom to add more *exotic* energy terms, not present in standard packages, to their simulations.

Tutorial TUT 2.2 Sun 16:45 HSZ 401
Micromagnetics simulations with MicroMagnum and OMNeS — •Kai Litzius and Matthias Sitte — Institute of Physics, Johannes Gutenberg-Universität, 55128 Mainz, Germany

The open-source micromagnetics simulator package MicroMagnum is a collaborative effort of the University of Hamburg and JGU Mainz. Based on the phenomenological Landau-Lifschitz-Gilbert equation, its core is intimately connected to experiments, aiding in their interpretation and analysis. In its current version, MicroMagnum comes with a complete set of modules to describe phenomenologically magnetic systems in terms of exchange interaction, magnetocristalline anisotropies,

external and magnetostatic fields, spin torques, etc. MicroMagnum has a robust and modular architecture that aims to combine the speed and flexibility of C++ together with the usability of the Python scripting language and allows to use both CPU- and GPU-based multithreaded computing, thereby gaining efficiency on regular grids compared to traditional packages such as OOMMF. It can be easily extended by the user through additional modules such as Dzyaloshinskii-Moriya interaction with arbitrary symmetries (to be released).

In the second part, we present OMNeS as a new, open source environment currently under development in the INSPIRE group at the JGU Mainz. OMNeS uses finite-element methods on unstructured grids as complementary approach to MicroMagnum, thereby allowing us to simulate large real-world devices capable of computing multiple device characteristics in a multi-scale and self-consistent manner.

15 min. break

Tutorial TUT 2.3 Sun 17:45 HSZ 401

Computational micromagnetics with JOOMMF — •Hans Fangohr and Marijan Beg — University of Southampton, SO17 1BJ, Southampton, United Kingdom

Computational micromagnetic studies complement experimental and theoretical studies, and are at times the only feasible way to address research challenges, effective industrial design and engineering of various products and systems. In this talk, we will introduce computational micromagnetics by using our Python interface to drive OOMMF, which is likely the most widely used micromagnetic simulation package. A major advantage of this interface is that OOMMF simulation runs are embedded in a general purpose programming language which enables the full use of the ecosystem of scientific libraries available for Python. For example, design optimisation, specialised post-processing, and visualisation can all be carried out in a single script, which significantly contributes to the reproducibility of micromagnetic research. This project is a part of the Jupyter-OOMMF (JOOMMF) activity in the OpenDreamKit project and we acknowledge financial support from Horizon 2020 European Research Infrastructures project (676541). The work is also supported by the EPSRC CDT in Next Generation Computational Modelling EP/L015382/1, and the EPSRC grants EP/M022668/1 and EP/N032128/1.

TUT 3: Tutorial: Patterns in Nature and Materials (DY/BP/CPP)

Pattern formation and self-organization in nature fascinates both the layman and reseachers from many disciplines. In addition to their aesthetic appeal, the function of the patterns in nature are of central interest. Therefore, function, variability and control of patterns are a focus of current research.

This tutorial is intended to give especially young scientists the opportunity to learn more about the subject of (nonlinear) pattern formation. Besides the introduction of fundamental and universal concepts in the field, examples from various disciplines of natural science and materials research will be presented.

Time: Sunday 16:00–18:30 Location: HSZ 04

Tutorial TUT 3.1 Sun 16:00 HSZ 04

The fascination of pattern formation: Basic principles, applications, future directions — •Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany

Self-organization and pattern formation are fundamental strategies in nature. In this talk I will give an introduction to the field and explain some main concepts with experiments. Using several examples from physics, biology or material science, I will illustrate that the mechanism driving a spatially extended pattern, like a stripe or traveling wave pattern, are vastly different in diverse systems. However, are there also common features in, for example, cloud streets, Turing patterns, wrinkles or stripes in active matter and fluids? I will explain that each nonlinear pattern has a number of robust and system-independent properties and that the concepts of pattern formation provide a theoretical framework for their generic properties. Why are patterns of different wavenumbers stable in homogeneous systems (variability)? By which generic principles can a pattern be selected or controlled? How do patterns interact with their environment such as boundaries or inhomogenities? Which functions do patterns in nature fulfill? Besides addressing these elementary questions, I will also highlight recent developments in the field, applications in emerging fields and possible future directions of pattern formation.

Tutorial TUT 3.2 Sun 16:50 HSZ 04

On growth and forms in nature — •Chaouqi Misbah — Laboratoire Interdisciplinaire de Physique, CNRS and Universite Alpes, Grenoble, France

Atoms and molecules self-assemble into fascinating patterns, such as snowflakes, that even very complex entities, such as biological cells and living micro-organisms, try to mimic despite their internal much higher complexity. This points to the existence of an intricate hierarchy of universality which still escapes today a comprehensive description. This lecture will present the basic rules and principles that lead to diverse non-equilibrium patterns and shapes in nature.

C. Misbah, Complex Dynamics and Morphogenesis: An Introduction to Nonlinear Science (Springer, 2016)

Tutorial TUT 3.3 Sun 17:40 HSZ 04

What can pattern formation theory tell us about ecosystem response to climate change? — •Ehud Meron — Ben-Gurion University, Beer-Sheva, Israel

Dryland landscapes show a variety of vegetation pattern-formation phenomena; banded vegetation on hill slopes and nearly hexagonal patterns of bare-soil gaps in grasslands are two striking examples. Vegetation pattern formation is a population-level mechanism to cope with water stress. It couples to other response mechanisms operating at lower and higher organization levels, such as phenotypic changes at the organism level and biodiversity changes at the community level, and plays a crucial role in understanding ecosystem response and ecosystem function in changing environments. In this talk I will present a platform of mathematical models for dryland ecosystems and describe some of the ecological questions we have studied using this platform. I will discuss the mechanisms that destabilize uniform vegetation and lead to periodic vegetation patterns, the variety of extended and localized patterns that can appear along a rainfall gradient, the impact of pattern-forming instabilities and front dynamics on state transitions (regime shifts), and restoration of degraded landscapes as a spatial resonance problem. I will conclude with a discussion of a major problem in our current era, the Anthropocene, namely, how to reconcile human intervention in ecosystems dynamics with ecological integrity.

E. Meron, Nonlinear Physics of Ecosystems, CRC Press 2015.

E. Meron, Pattern formation – A missing link in the study of ecosystem response to environmental changes, Mathematical Biosciences 271, 1 (2016).

TUT 4: Tutorial: Photocatalysis (HL/O)

Time: Sunday 16:00–18:15 Location: HSZ 403

Tutorial TUT 4.1 Sun 16:00 HSZ 403

An Introduction to Rechargeable Battery Technology and Current Research Trends — •Bryan McCloskey — Department of Chemical and Biomolecular Engineering, UC, Berkeley, CA, USA — Energy Storage and Distributed Resources Division, LBNL, Berkeley, CA, USA

From electric and plug-in hybrid vehicles gaining a foothold in the automotive market to the 787 airline and Galaxy Note 7 battery fires, battery technology has, for better or worse, found itself in the popular spotlight in recent years. This spotlight is likely to shine brighter in the future, as improvements in both capability and size of portable electronic devices will make batteries and battery research increasingly important in the coming decade. Nevertheless, the 787 and Galaxy Note 7 incidents highlight an interesting dichotomy in battery research: although decades of development have allowed rechargeable batteries to be used in advanced applications, our understanding of how to design a safe, high energy density, low cost rechargeable battery still needs to be improved. This talk will initially give a general introduction to battery technology, including Li-ion batteries, focusing on their chemistry and applications. The second part of the talk will outline research directions associated with improving rechargeable batteries, with a specific emphasis on research activities for advanced materials development, including solid-state batteries and the so-called *beyond Li-ion* chemistries (Li-S, Li-air (O2), and Mg-ion batteries).

Tutorial TUT 4.2 Sun 16:40 HSZ 403

Theory and Simulations for All-Solid State Batteries — •Christoph Scheurer — Theoretische Chemie, TU München, Lichtenbergstr. 4, 85748 Garching, Germany

The concept of an All-Solid State Battery (SSB) has recently attracted substantial interest for its potential advantages over conventional liquid electrolyte-based batteries, which are slowly approaching their fundamental limitations. The SSB is often considered inherently safe due to the intrinsic separator function of solid electrolytes, as well as longterm stable, being based exclusively on solid inorganic or polymer electrolytes and electrodes and thus avoiding the use of potentially volatile and flammable organic solvents. The lack of a liquid electrolyte, on the other hand, also poses several challenges like e.g. interfacial resistances or mechanical stress and contact loss at solid-solid interfaces, which need to be fully understood and overcome for a functional, competitive SSB.

In this tutorial we will discuss key topics within the theory of superionic and mixed ionic-electronic conductors to understand the requirements for solid state electrolytes, electrode materials and their interplay. Traditional electrochemical concepts will be connected to recent atomistic simulations employing density functional theory (DFT) electronic structure, force-field based molecular dynamics (MD) and Monte-Carlo (MC), as well as coarse-grained kinetic Monte-Carlo (kMC) computations.

Coffee Break

Tutorial TUT 4.3 Sun 17:35 HSZ 403

Solid State Ionics - Mechanisms and Experimental Methods in Battery Research — •Ruediger-A. Eichel — Forschungszentrum Juelich, Institut fuer Energie- und Klimaforschung — RWTH Aachen, Institut fuer Physikalische Chemie

Solid-State Batteries promise safe, long-lived, high volumetric energy density and easily miniaturized (as thin films) devices for energy storage. However, because high currents generally only cross solid-solid interfaces at high transition resistances, current solid-state batteries mainly are limited to low-power densities.

In this contribution, the underlying principles of Solid-State Ionics, i.e. the foundations of charge transport and transfer in the 'bulk' and accross boundaries, are outlined together with an introduction of the most prominent experimental techniques for characterization of these phenomena and mechanisms. Furthermore, recent examples of application in the field of Solid-State Batteries are outlined.