TUT 1: Creating and Running Automated Workflows for Material Science Simulations (joint session MM/TUT)

Time: Sunday 16:00–18:30 Location: H 0104

Tutorial TUT 1.1 Sun 16:00 H 0104

Hands-on tutorial: Creating and running automated workflows for materials science simulations — •Jörg Neugebauer[1], Tilmann Hickel[1,2], and Ralf Drautz[3] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf — [2]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin — [3]ICAMS Ruhr-Universität Bochum, Bochum

Advanced computational simulations in materials science have reached a maturity that allows one to accurately describe and predict materials properties and processes. The underlying simulation tasks often involve several different models and software that require expert knowledge to set up a project and to vary input parameters. The accompanying increasing complexity of simulation protocols means that the workflow along the simulation chain becomes an integral part of research. Effective workflow management therefore is important for efficient research and transparent and reproducible results as also highlighted in the NFDI-MatWerk initiative. In this hands-on tutorial we will provide an interactive hands-on introduction into managing workflows with pyiron (www.pyiron.org). Pyiron is an integrated development environment for materials science built on python and Jupyter notebooks that may be used for a wide variety of simulation tasks, from rapid prototyping to high performance computing. The tutorial will give a general introduction to using pyiron, with a focus on atomistic simulation tasks, followed by the construction of fully ab initio phase diagrams obtained by the training and validation of ACE-machine learning potentials providing a real-life application example.

TUT 2: Dynamics of Economic and Financial Systems (joint session SOE/TUT)

This tutorial is aimed to introduce concepts and illustrate latest developments on the dynamics of economic and financial systems: non-stationary dynamics of correlations in financial markets, interpretable machine learning applied to electricity price dynamics in the context of transitioning to sustainable energy sources, and financial concepts connecting statistical physics and financial markets.

Participants are invited to continue the deep dive into the above topics at the symposium "Statistical Physics of Economic and Financial Systems (SYEF)" on Thursday at 9:30 (Audimax).

Organized by Eckehard Olbrich (Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany), Fakhteh Ghanbarnejad (Potsdam Institute for Climate Impact Research, Potsdam, Germany), and Philipp Hövel (Saarland University, Germany)

Time: Sunday 16:00–18:15 Location: H 1012

Tutorial TUT 2.1 Sun 16:00 H 1012

Non-Stationary Dynamics of Correlations in Financial Markets — •Anton J. Heckens — Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg

Financial markets are strongly correlated complex systems. The internal processes in the markets constantly change, and the external effects on the markets do change as well. This implies that there is no form of equilibrium whatsoever, rather, the financial markets are highly non-stationary. This has a large impact also on the correlations of stock prices. Here, I focus on the non-stationarity of the correlation structure that the market as a whole shows. Obviously, systemic risk and its management are severely affected. However, the non-stationarity itself has a structure because quasi-stationary states emerge, disappear, reemerge. They are the different operational modes of the market, reflecting various changes and restructurings. I will give an overview of data-driven research in this field of econophysics for a general audience interested in complex systems, not exclusively for experts.

Tutorial TUT 2.2 Sun 16:45 H 1012

Exploring electricity price dynamics with interpretable machine learning — •Benjamin Schäfer[1] and Dirk Witthaut[2] — [1]Karlsruhe Institute of Technology (KIT) — [2]Research Center Jülich (FZJ)

Mitigation of climate change requires a fundamental transformation of our energy system. Power plants based on fossil fuels must be replaced by renewable power sources, such as wind and solar power. This energy transition (Energiewende) towards a sustainable energy system raises numerous complex challenges, as power generation becomes more uncertain, while simultaneously more operational data becomes available. Hence, data-driven approaches have become feasible and even necessary to fully understand the energy systems of today and tomorrow across all scales.

Machine learning and artificial intelligence can handle these enormous amounts of data but need to do so in a transparent way. Obtaining classifications or forecasts without explanations limits their use severely.

Within this tutorial, we will discuss the uses of machine learning in energy systems and review approaches to make initial 'black box' models transparent. As an application, we will consider electricity markets and price dynamics.

Tutorial TUT 2.3 Sun 17:30 H 1012

Rien ne va plus: Seemingly perfect bets and optimal portfolios, broken ergodicity, washed-out stylized facts and financial death by Black-Scholes option pricing — •Jan Nagler — Centre for Human and Machine Intelligence, Frankfurt

Let's walk the line, together, in this tutorial: From Kelly-optimal bets, blindfolded trading, volatility drag, and ergodicity, to universal power laws in financial markets. On the electronic blackboard, we will develop concepts in statistical physics suited for our guaranteed financial ruin, chasing a fundamental understanding of some concepts and how they are linked together.

TUT 3: Exploring Ferroic Materials: From Modelling to Imaging Techniques (joint session KFM/TUT)

Recent developments in the study of ferroic materials have unveiled exciting features, encompassing phenomena such as skyrmions and multiferroic domain walls. This tutorial seeks to provide a comprehensive overview, spanning from fundamental theoretical concepts to advanced imaging techniques. We will learn how these cutting-edge developments now enable the bridging of length scales from the individual atom to the macroscopic understanding of the ferroic ordering.

Organizer: Felix Büttner (Univ. Augsburg), Jan Schultheiß (Univ. of Canterbury) Session Chairs: John Freeland (Argonne National Lab), Manuel Zahn (Univ. Augsburg)

Time: Sunday 16:00–18:15 Location: H 1028

Tutorial TUT 3.1 Sun 16:00 H 1028

Ferroelectric domains, domain walls, symmetry and thermodynamic models — •Jiri Hlinka — Institute of Physics, Czech Acad. Sci., Prague, Czechia

Properties and applications of the materials with ferroelectric or other kind of ferroic domains separated by domain walls continue to stimulate our desire to image, model and understand these ultimate nanoscale interfaces in more and more details. We aim to present here only the most general theoretical concepts that can be useful in related physics and materials science activities. In this tutorial presentation, also aimed to facilitate the most recent achievements presented at the DPG meeting, we intend to cover the subject mostly from the phenomenological point of view, relying on the symmetry constraints and Ginzburg-Landau theory arguments.

Tutorial TUT 3.2 Sun 16:30 H 1028

Nanoscale ferroelectricity: insights from optical second harmonic generation — •Nives Strkalj — Institute of Physics, Zagreb

Ferroelectric materials are a promising platform for energy-efficient electronic and optical devices. In thin films, relevant for applications, ferroelectricity is highly susceptible to the influence of interfaces through electrostatic and elastic boundary conditions. A large surface-to-volume ratio at the nanoscale thus leads to dramatic changes in polarization direction, magnitude, and domain configuration. However, evaluating ferroelectricity in thin films remains a challenge for conventional techniques because of significant non-ferroelectric contributions. A highly sensitive optical method, second harmonic generation (SHG), can be used to detect polarization in thin films. SHG has thus become an invaluable tool for studying size effects in nanoscale ferroelectrics.

In my talk, I will give an introduction to ferroelectricity, ferroelectric size effects, and approaches to tuning polarization in nanoscale films. I will present insights from SHG into the emergence and evolution of ferroelectricity in thin films. Finally, I will address the use of SHG for tracking polarization during the growth process - in situ - to access transient effects. I will conclude by showing examples of harnessing findings from SHG to engineer desired ferroelectric responses for specific applications.

15 min. break

Tutorial TUT 3.3 Sun 17:15 H 1028

Magnetic imaging with solid-state spin defects — •Vincent Jacques — Laboratoire Charles Coulomb, CNRS and Uni. Montpellier, France

Experimental methods enabling the optical detection of single spins in the solid-state, which were initially developed for quantum information science, open new avenues for the development of highly sensitive quantum sensors. In this context, the electronic spin of a single nitrogen-vacancy (NV) defect in diamond can be used as an atomic-sized magnetometer, providing an unprecedented combination of spatial resolution and magnetic sensitivity, even under ambient conditions. In this talk, I will first introduce the principle of scanning-NV magnetometry and discuss how it can be used as a powerful tool for exploring the physics of ferroic materials. I will then discuss recent efforts in researching alternative material platforms that could expand the range of quantum sensing functionalities offered by diamond, with a focus on hexagonal boron nitride.

Tutorial TUT 3.4 Sun 17:45 H 1028

Exploring Ferroic Materials in 3D using Atom Probe Tomography — •Shelly Conroy — Department of Materials, London Centre for Nanotechnology, Imperial College London, London SW7 2AZ, UK

Ferroic materials can contain complex interfaces such as grain boundaries, dislocations, domain walls, and higher order topologies. Even slight changes in chemical composition can result in drastic changes in functionality such as conductivity and magnetism. As the regions of interest are often only a unit cell thick and can meander throughout the bulk material in 3D it is vital to have a characterisation method that can achieve the required spatial resolution in 3D. Atom probe tomography (APT) provides 3D compositional mapping of materials with sub-nanometre spatial resolution. In this tutorial the basics of APT characterisation will be discussed, including how to make samples, how to process APT data and specific examples of APT analysis of ferroic materials. Additionally correlative electron microscopy techniques will be detailed, and how to combine structural with chemical information from both techniques.

TUT 4: Thermoelectricity – Fundamental Aspects, Materials, Applications (joint session TT/TUT/MA)

Thermoelectric effects have been discussed for several decades and have found widespread applications. Characteristic physical quantities are the efficiency, the figure of merit, ZT, and the power factor. In particular, increasing ZT has been the issue for many years. In recent developments, the focus has been on "unconventional" thermoelectric phenomena and materials: these include, in particular, transverse thermoelectric effects where the generated charge current is perpendicular to the temperature gradient, as can be observed, e.g., when applying a magnetic field (ordinary and anomalous Nernst effect). Transverse thermoelectricity can be found even without a magnetic field, e.g., in goniopolar materials (which have n- and p-type parts of the Fermi surface at the same time). – The Tutorial, jointly organized by the divisions MA and TT, will cover the basic physics of thermoelectricity, as well as discuss the question which materials are most useful for which applications, respectively. Attending the Tutorial thus will allow the non-experts in the field to fully appreciate the related presentations in the conference.

Organizers: Ulrich Eckern (University of Augsburg), Claudia Felser (MPI CPS Dresden), Anke Weidenkaff (TU Darmstadt & Fraunhofer IWKS)

Time: Sunday 16:00–18:10 Location: H 1058

Tutorial TUT 4.1 Sun 16:00 H 1058
Transport properties of thermoelectric materials — •Maria Ibáñez — Institute of Science and Technology (ISTA), Klosterneuburg, Austria

Thermoelectricity is the phenomenon of converting heat directly into electricity and vice versa. As energy harvesters, thermoelectric devices can be used to partially recover large quantities of the waste heat to reduce our primary energy production or to run low-power devices, especially those that require autonomy, such as sensors and transmitters in remote or difficult-to-access locations. Furthermore, its reversible nature allows thermoelectric devices to be operated as precise coolers for small-scale temperature control. Such localized cooling is crucial in infrared detectors, microelectronics, and optoelectronics, among others, where space is limited, and heat dissipation is localized. This lecture will provide a comprehensive introduction to thermoelectricity. We will begin by giving a brief history of thermoelectrics, a description of the phenomenon, and its potential applications. Later on, we will introduce the fundamental principles of thermoelectricity, emphasizing the importance of material properties, in particular, those related to electronic and thermal transport. We will present the thermoelectric figure of merit and its significance as a metric for evaluating thermoelectric efficiency. ZT components, including electrical conductivity, Seebeck coefficient, and thermal conductivity, and their interplay in determining the overall performance will be deeply evaluated, and the different strategies to maximize performance will be presented using, as examples, traditional thermoelectric materials.

5 min. break

Tutorial TUT 4.2 Sun 16:45 H 1058
Thermoelectricity: basic concepts, and applications to nanoscale heat engines — •Karol I. Wysokiński — Institute of Physics, M. Curie-Sklodowska University, Lublin, Poland

Thermoelectric power generators directly convert heat into electricity. These solid-state heat engines have no moving parts and are extremely reliable. Their performance is characterized by efficiency and power output, both of which depend on a single parameter called the thermoelectric figure of merit ZT, of which they are monotonically increasing functions. The dimensionless parameter ZT depends on the materials' transport coefficients: conductivity, thermal conductivity, Seebeck coefficient, and operating temperature. However, due to the coupling between conductivity and thermal conductivity quantified by the Wiedemann-Franz ratio obeyed by standard materials, the quest to increase ZT is a challenge for contemporary materials physics. Novel materials and structures have been proposed to overcome these difficulties on the way to achieve efficient waste heat harvesters with possible applications at large and small scales.

During the lecture, the above main ideas in the theory of thermoelectricity will be discussed, and their application in the nanoscale illustrated by the analysis of the devices consisting of a single or two quantum dots, tunnel coupled to two or more external electrodes. The electrodes may be simple metals, ferromagnets, or superconductors. The steady-state transport characteristics of the devices will be analysed. Special attention will be paid to the role of interactions between the carriers, and the non-linear effects prevalent in such structures.

5 min. break

Tutorial TUT 4.3 Sun 17:30 H 1058
Novel thermoelectric materials: synthesis, characterization and application — •Wenjie Xie — Institute of Materials Science, Technical University of Darmstadt, Darmstadt, Germany — Fraunhofer IWKS, Alzenau, Germany

Thermoelectricity offers a direct and highly efficient approach for converting heat into electricity, relying on two key factors: Carnot efficiency and the materials-dependent property, ZT. Over the past two decades, significant progress has been made in pursuing high ZT thermoelectric materials, culminating in a bulk ZT surpassing 3. In this presentation, we offer a comprehensive review of the development of novel thermoelectric materials, categorized according to their application temperature ranges: low/room, medium, and high temperatures.

Within each temperature range, we will focus on the synthesis and characterization of one or two exemplary materials. For instance, the discussion will delve into materials such as Bi_2Te_3 for room temperature applications, SnSe/PbTe for medium temperature regimes, and the utilization of half-Heusler and oxide materials for high-temperature scenarios. Furthermore, the sustainable aspects of thermoelectric material synthesis will be explored.

Last, we will discuss the practical application of thermoelectric materials, examining their usage in real-world scenarios. The discussion will mainly focus on Bi_2Te_3, half-Heusler, and oxides, providing a comprehensive overview of the current landscape and future potential in the realm of thermoelectric cooling and power generation.

TUT 5: FAIR Research Data – Generation, Handling and Analysis within the FAIRmat Infrastructure

In many scientific fields, but especially in solid-state physics, comprehensive and homogeneous scientific data could pave the way for a completely new, data-driven research, often referred to as the fourth paradigm of science. New opportunities for science and technology, as well as for teaching and career paths are foreseeable. In reality, however, our field mostly provides extremely heterogeneous data. For this reason, the major funding organizations are calling for and supporting the conversion to FAIR (findable, accessible, interoperable, reusable) data. In solid-state physics, the consortium FAIRmat aims at developing concepts and solutions for this endeavor. This tutorial introduces the FAIRmat approach in four well-adapted contributions.

Organizers: Martin Aeschlimann (TU Kaiserslautern) and Laurenz Rettig (FHI Berlin)

Time: Sunday 16:00–18:15 Location: H 2013

Tutorial TUT 5.1 Sun 16:00 H 2013

Experimental research data as a FAIR resource: Introduction and the FAIRmat approach — •Heiko B. Weber — Lehrstuhl für Angewandte Physik, Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

I will introduce the general framework of research data management and give an overview of FAIRmat's concepts on how to implement it in experimental solid-state physics. I will sketch how research data (collected by instruments) and metadata (collected in electronic laboratory notebooks and from instruments) can be consistently structured. Such harmonized data can be collected in local or worldwide hubs (NOMAD Oasis or NOMAD, respectively). On this platform one can search data, work with the data, compare data of different origin, and finally use it as repository. Implications for science and teaching, and for the solid-state physics community will be briefly discussed.

Tutorial TUT 5.2 Sun 16:30 H 2013

Harmonization concepts for experimental research data: NOMAD and NeXus — •Sandor Brockhauser — Physics Department and CSMB, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

In order to achieve interoperability for data of different origin, a FAIR research-data platform for solid-state physics is created within FAIRmat, which we term NOMAD. It features flexible, but structured data modeling, allows custom data ingestion, while providing efficient search capabilities and online visualization of datasets. Several standard data formats are supported by NOMAD including the NeXus format [1].

In this tutorial, I will introduce NeXus as a community-driven data modeling standard for experiments. I will present the NeXus Ontology and discuss several examples of how a specific experimental community can extend it to cover their special needs. Finally, the integration of NeXus data from experiments into NOMAD will be introduced.

[1] https://www.nexusformat.org/

Tutorial TUT 5.3 Sun 17:00 H 2013

How to build FAIR data pipelines for photoemission spectroscopy — •Florian Dobener — Physics Department and CSMB, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — Physics Department & Research Center OPTIMAS, RPTU Kaiserslautern, Germany

Photoemission spectroscopy (PES) is presented as a use case for pioneering future research data concepts. We will show how FAIR research data can be organized and how we intend to create benefits for the scientists who participate. We will present an extensive and elaborated standard (NXmpes) for harmonizing PES data using NeXus. This tutorial aims to provide comprehensive guidance on how to establish a FAIR data pipeline within your laboratory using NXmpes in conjunction with the NOMAD research data management platform.

Our tooling integrates seamlessly with NOMAD's data management capabilities. Alternatively, it offers standalone tools for generating NXmpes files, facilitating their incorporation into custom data generation pipelines. Moreover, we present our strategy to collaborate with leading manufacturers of PES equipment to foster interoperability of NXmpes with their software solutions.

Tutorial TUT 5.4 Sun 17:30 H 2013

Easy access to FAIR data generation for custom-built experiments with NOMAD CAMELS — •Alexander Fuchs — Lehrstuhl für Angewandte Physik, Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — Physics Department and CSMB, Humboldt-Universität zu Berlin, Germany

In this tutorial, I will introduce NOMAD CAMELS [1] as a standalone open-source measurement software targeted towards the requirements of experimental physics. It is designed to control instruments and to write and modify experimental procedures without the need of programming skills. CAMELS creates python code, which subsequently runs the measurement protocol, hence it can utilize powerful libraries and is widely extendable. CAMELS provides by default rich metadata and structured research data in a consistent way. With its NeXus output, immediate injection of FAIR data into NOMAD Oasis and NOMAD will be possible.

In this tutorial, I will explain the concept and capabilities of CAMELS, take the beginner's perspective and demonstrate how to start using it.

[1] https://nomad-lab.eu/nomad-lab/nomad-camels.html

Q & A with all Presenters (15 min.)