TUT 1: Tutorial: Thermoelectricity - The Quest for a High Figure of Merit (TT)

The search for and the investigation of novel materials with excellent thermoelectric properties, i.e., a high "figure of merit", has been a hot topic recently, in particular, in view of numerous technological applications. For example, a greater efficiency would generate brand new possibilities in the field of power engineering, by using directly the waste heat in combustion engines while lowering CO_2 emissions at the same time, or in energy self-sufficient sensors. In this Tutorial, after an introduction into the basic theoretical concepts, measurements at the nanoscale will be discussed, as well as applications in power generators.

Organizers: Ulrich Eckern (Uni Augsburg), Claudia Felser (MPI CPfS Dresden)

Time: Sunday 16:00–18:25 Location: HSZ 304

Tutorial TUT 1.1 Sun 16:00 HSZ 304
Thermoelectric Effects: Basic Aspects, Boltzmann Theory, Onsager Relations — •Arthur Ernst — Max-Planck-Institut für Mikrostrukturphysik, Halle — Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig

Thermoelectric phenomena which involve the conversion between thermal and electrical energy and provide a method of heating and cooling materials are expected to play an important role in meeting the energy challenge of the future. In my talk I shall present basic aspects of the microscopic theory for thermoelectricity. First, I discuss the basic definition of the thermoelectric heat. Then I present a short overview of non-equilibrium thermodynamics and the microscopic theory of the electronic transport. Further I review several approaches to describe thermoelectric properties, present the state of the art in the understanding the thermoelectric phenomena, and conclude my talk with some remarks on future prospects of the field.

5 min. break

Tutorial TUT 1.2 Sun 16:50 HSZ 304
Thermal Transport Measurements at the Nanoscale — •Saskia F. Fischer — AG Neue Materialien, Humboldt-Universität zu Berlin, 10099 Berlin

In this tutorial first an introduction to measurements of the electrical conductivity, the thermopower and the thermal conductance will be given. All three material parameters are required to determine the thermoelectric figure of merit. However, the measurement techniques which are successfully applied to bulk materials often cannot be transferred to nanoscale materials such as individual ultra-thin films, flakes or nanowires. On behalf of particular examples, I will discuss measurement techniques for such nanomaterials. In particular, the application of a micro-machined platform for the full ZT-characterization allowing as well for the investigation of the crystal structure and chemical composition of a single nanowire will be demonstrated. If time allows, an outlook to thermal transport in low-dimensional charge carrier systems and the determination of the charge carrier temperature via noise thermometry will be given.

5 min. break

Tutorial TUT 1.3 Sun 17:40 HSZ 304
High Temperature Thermoelectric Power Generators: Materials and Devices — •Anke Weidenkaff[1,2] and Wenjie Xie[2] — [1]Empa, 8600 Dübendorf, Switzerland — [2]Institut für Materialwissenschaft, Universität Stuttgart, 70174 Stuttgart, Germany

With a thermoelectric converter heat can be directly converted into electricity. A broad application of thermoelectric converters in future energy technologies requires the development of thermoelectric active, stable, low cost and sustainable materials. Suitable candidates are being selected among novel materials according to their temperature dependent ZT (thermoelectric figure of merit) values, and their compatibility factors to produce well performing thermoelectric converters, delivering a high power output. Theses converters are tested under ambient air at temperatures of $T > 900$ °C and applied in an exhaust gas stream of a custom made hybrid vehicle, concentrated solar thermal converters, metal casting furnaces and solid oxide fuel cells. The lectures will provide an overview on the development of novel perovskite-type and Heusler materials gaining importance for future energy technologies

TUT 2: Tutorial: Advanced Algorithms for Correlated Quantum Matter (TT)

This Tutorial provides an introduction into a most important sub-field of computational physics, namely the investigation of strongly correlated quantum systems by modern numerical methods. Further details and recent scientific advancements will be presented in the corresponding TT Focus Session (Tuesday, starting at 9:30 in HSZ 03).

Organizers: Fakher Assaad (Uni Würzburg), Ulrich Eckern (Uni Augsburg)

Time: Sunday 16:00–18:25 Location: HSZ 04

Tutorial TUT 2.1 Sun 16:00 HSZ 04
DMRG and Entanglement Scaling — •Fabian Heidrich-Meisner — Ludwig-Maximilians-University Munich, Germany

This talk will provide an introduction to the density matrix renormalization group method which provides numerical access to many-body wave functions of quantum lattice models such as the Hubbard, Heisenberg, or the t-J model. The main idea is to approximate wave-functions through finite-dimensional matrix product states (MPS). The performance of the technique is intimately related to the entanglement encoded in the target wave-function. For gapped Hamiltonians with short range interactions, the so-called area law states that their ground states are only mildly entangled, permitting an efficient representation of many-body states using MPS in one dimension. The more difficult case of two-dimensional systems, critical systems in one dimension, and time-evolution will also be discussed.

5 min. break

Tutorial TUT 2.2 Sun 16:50 HSZ 04
Introduction to Tensor Networks — •Roman Orus — Institut für Physik, Johannes Gutenberg Universität, Staudingerweg 7, 55099 Mainz, Deutschland

In this tutorial I will give an introduction to Tensor Network methods for strongly correlated systems. Motivated by DMRG and the entanglement properties of 1d systems (see the related previous tutorial), I will extend the ideas to deal with other types of situations, such as 2d and scale-invariant systems. The PEPS and MERA tensor networks will be presented and discussed. After providing practical examples, I will explain some of the related numerical methods at an introductory level.

5 min. break

Tutorial TUT 2.3 Sun 17:40 HSZ 04
Quantum Monte Carlo Methods — •Stefan Wessel — Institute for Theoretical Solid State Physics, RWTH Aachen University, Aachen, Germany

This tutorial will introduce the basic ideas behind modern quantum Monte Carlo simulation methods, focusing on world-line approaches for quantum spin systems. In particular, the cluster-based loop algorithm in the continuous-time formulation as well as the stochastic series expansion and the directed loop update approach will be presented. The advantages and limitations of these simulations methods will be discussed.

TUT 3: Tutorial: Non-equilibrium dynamics (AGjDPG with DY)

Classical thermodynamics deals with systems in (quasi) equilibrium. However, due to external energy supply or removal a system can be driven out of equilibrium. As a consequence the behavior of these systems differs in several respects from those in classical thermodynamics.

This tutorial is intended to give especially young scientists the opportunity to learn more about the subject of non-equilibrium processes. Besides the introduction to some fundamental concepts several example systems will be discussed.

Time: Sunday 16:00–18:15 Location: HSZ 105

Tutorial TUT 3.1 Sun 16:00 HSZ 105
Nonlinear deterministic and nonlinear stochastic processes as models in non-equilibrium physics — •Holger Kantz — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Due to friction, every macroscopic system eventually enters a rest state unless it is externally driven. Whereas purely constant or periodic driving leads us to deterministic models, additional coupling to a heat bath results in non-equilibrium stochastic processes. This tutorial, to be understood in conjunction with the two other talks given by H. Stark and U. Seiffert, tries to cover the most relevant and most striking aspects of low-dimensional deterministic and stochastic dynamics of driven systems: bifurcations, lack of a superposition principle, self-organisation, and the interpretation as an entropy producing/exporting system.

Tutorial TUT 3.2 Sun 16:45 HSZ 105
Stochastic Thermodynamics — •Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, Germany

In this talk, I will give an introduction to the emerging field of stochastic thermodynamics and illustrate its main concepts with recent experimental data. Stochastic thermodynamics provides a framework for describing small systems embedded in a heat bath and externally driven to non-equilibrium [1]. Examples are colloidal particles in time-dependent optical traps, single biomolecules manipulated by optical tweezers or AFM tips, and motor proteins driven by ATP excess. The notions of classical thermodynamics like applied work, exchanged heat and total entropy production valid there on the ensemble level can now be consistently identified and measured on the level of an individual stochastic trajectory. Moreover, exact results that refine the second law like the Jarzynski relation and fluctuation theorems for entropy production can be proven. Using these concepts, the efficiency of nanoscopic machines like molecular motors can be determined and their performance be optimized.

[1] U. Seifert, Rep. Prog. Phys. 75, 126001, 2012.

Tutorial TUT 3.3 Sun 17:30 HSZ 105
Active motion at low Reynolds number — •Holger Stark — Institut für Theoretische Physik, TU Berlin, D-10623 Berlin, Germany

Starlings over Rome form dynamic swarms, fishes in water move collectively in fish schools. Zooming from the macroscopic into the microscopic world, bacteria also show intricate collective behavior.

However, on the micron scale swimming in aqueous environment requires different strategies than in the macroscopic world since at low Reynolds number drifting by inertia is not possible. Biological swimmers like bacteria and artificial microswimmers constantly consume energy to move forward. They are always in nonequilibrium.

The talk demonstrates some swimming strategies from nature but also of man-made microswimmers. It then illustrates at a few examples, how active motion reveals itself already on the single-swimmer level but also in the collective properties when many swimmers interact.

TUT 4: Tutorial: Festkörpercharakterisierung mit Positronen (MI)

Die Positronenannihilation hat sich seit einigen Jahrzehnten als Methode zur Untersuchung der Real- und Elektronenstruktur von kristallinen Festkörpern bewährt. Positronen, die in Strukturdefekten eingefangen werden (Leerstellen, Leerstellencluster, Versetzungen, Korngrenzen, Ausscheidungen) ändern ihre Annihilationsparameter, so dass Aussagen zur Art und Dichte der Defekte getroffen werden können. In den letzten Jahren ist eine weitere Anwendung in dielektrischen Stoffen hinzugekommen: hier bildet sich Positronium, dessen Lebensdauer ein Maß für das offene Volumen in der Probe ist. So kann bspw. das Volumen zwischen Polymerketten oder Porengrößen in Mikro- und Mesoporen charakterisiert werden. In den drei Tutorial-Vorträgen werden diese Aspekte näher erläutert. Weiterhin werden die beiden Nutzeranlagen für alle Aspekte der Positronenannihilation am FRM-II und an ELBE (HZDR) detailliert vorgestellt. Es wird erläutert, wie man als externer Nutzer Strahlzeit erhalten kann.

Chair: R. Krause-Rehberg (Martin-Luther-Universität Halle-Wittenberg)

Time: Sunday 16:00–18:15 Location: HSZ 201

Tutorial TUT 4.1 Sun 16:00 HSZ 201
Positrons probing matter: What we learn about lattice defects and electronic structure using positron beams — •Christoph Hugenschmidt — E21 Physik-Department und FRM II, Technische Universität München, Lichtenbergstraße 1, 85747 Garching

Monoenergetic positrons beams are applied in a large variety of experiments in solid state physics and material science. Examples are spatially resolved defect maps of plastically deformed or irradiated metals, non-destructive investigation of layered systems, the annealing behaviour of defects or the free volume in polymers. At the surface, the annihilation of positrons with core electrons initiates the emission of Auger-electrons that allows the examination of the topmost atomic layer. In addition, the electronic structure such as anisotropies of the Fermi surface can be studied too.

Within this contribution the basic properties of positron annihilation studies will be explained. The benefit of positron beam experiments will be elucidated by selected experiments, such as (i) defect sensitive positron lifetime experiments, (ii) elemental selective (coincident) Doppler broadening spectroscopy of the annihilation line, (iii) angular correlation of annihilation radiation experiments, and (iv) time-dependent positron annihilation induced Auger-electron spectroscopy.

The neutron induced positron source NEPOMUC provides the world's highest intensity of more than 10^9 moderated positrons per second. An overview of the NEPOMUC beam facility and the positron instrumentation is given and future developments and applications of the high-intensity positron beam will be discussed.

Tutorial TUT 4.2 Sun 16:45 HSZ 201

Theoretical electron and electron-positron momentum densities of transition metals and their compounds in the presence of many-body correlation effects — •Liviu Chioncel — Theoretische Physik III, Zentrum für Elektronische Korrelationen und Magnetismus Institut für Physik Universität Augsburg — Augsburg Center for Innovative Technology

Valuable information about the nature of many-electron interactions in transition metals and their compounds is obtained from experiments based on Compton and positron annihilation spectroscopy the later especially in the form of angular correlation of annihilation radiation measurements. These experiments access the electron momentum density and the momentum density of annihilating electron-positron pairs. Here we review theoretical state of the art techniques that combine Density Functional and Dynamical Mean Field Theory which allows to calculate the electron momentum densities. We survey recent experiments and calculations for paramagnetic and ferromagnetic transition metals and half-metallic ferromagnets.

Tutorial TUT 4.3 Sun 17:30 HSZ 201

Positron annihilation studies at an electron accelerator: From thin films to bulk samples and 3-D imaging — •Andreas Wagner — Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany

Positron annihilation lifetime spectroscopy serves as a perfect tool for studies of open-volume defects in solid materials such as vacancies, vacancy agglomerates, and dislocations. Moreover, structures in porous media can be investigated ranging from 0.3 nm to 30 nm employing the variation of the positronium lifetime with the pore size. While lifetime measurements close to the material's surface can be performed at positron-beam installations, bulk materials, fluids, gases, bio-materials or composite structures cannot or only destructively accessed by positron beams. In the tutorial, a set of new installations at the superconducting electron linear accelerator ELBE will be discussed. Key to all experiments is the timing resolution and the variability in pulse repetition rate which enables new ways of materials research with positrons. Depth dependent defect studies (both annihilation lifetime and Doppler-broadening) on thin films are enabled by a tunable monoenergetic positron beam. Experiments using high-energy electron-bremsstrahlung as a source for pair production inside the investigated samples release vacuum constraints and allow studying structural defects on the atomic scale even for radioactive samples with significant intrinsic activities. Some recent examples and results will be given and a facility extension for in-situ defect generation studies will be presented.

TUT 5: Tutorial: Energy materials (HL with MA)

This tutorial introduces basic physical concepts underlying the microscopic working principles of a broad and diverse range of energy materials ranging from organic solar cells to strong magnets for wind turbines. Leading scientists from various different disciplines – both from academia and industry – will give an exciting overview of the state-of-the art in their specific field of expertise. The topics to be covered include: Electrochemical energy storage and battery research, superstrong magnets and magnetocalorics, dye-sensitized solar cells from the Graetzel cell to hybrid inorganic-organic perovskites, and solar water splitting. We also refer to the parallelly running tutorial on thermoelectricity. All talks are specifically prepared for a broad audience.

Organized by Erich Runge, TU Ilmenau, and Christoph Lienau, Carl von Ossietzky Universität Oldenburg, on behalf of the Semiconductor Physics Division jointly with the Magnetism Division.

Time: Sunday 16:00–18:35 Location: HSZ 403

Invited Talk TUT 5.1 Sun 16:00 HSZ 403

Von Lithium zu Lithium-Ionen-Batterien und zurück — •Martin Winter — WWU Münster, Deutschland

Invited Talk TUT 5.2 Sun 16:35 HSZ 403

Magnetic materials for green energy applications — •Oliver Gutfleisch — TU Darmstadt, Material Science, Functional Materials — Fraunhofer Project Group Materials Recycling and Resource Strategy IWKS

Due to their ubiquity, magnetic materials play an important role in improving the efficiency and performance of devices in electric power generation, conversion and transportation 1. Permanent magnets are essential components in motors and generators of hybrid and electric cars, wind turbines, etc. Magnetocaloric materials could be the basis for a solid state energy efficient cooling technique alternative to compressor based refrigeration. Any improvements in magnetic materials will have a significant impact in these areas, on par with many *hot* energy materials efforts (e.g. hydrogen storage, batteries, thermoelectrics, etc.).

The talk focuses on rare earth and rare earth free permanent magnet and magnetocaloric materials with an emphasis on their optimization for energy and resource efficiency in terms of the usage of critical elements. The synthesis, characterization, and property evaluation of the materials will be examined briefly having in mind their critical micromagnetic length scales and phase transition characteristics.

Coffee break (10 min.)

Invited Talk TUT 5.3 Sun 17:20 HSZ 403

Recent developments of dye sensitized and mesoscopic solar cells — •Toby Meyer — Solaronix SA, Aubonne, Switzerland

The latest results on the Dye Sensitized Solar Cell developments at Solaronix are presented in the international context, both scientifically and economically. Examples include the first application in a 250 m^2 vertical façade at the Swisstech Convention Center (EPFL, Lausanne). Furthermore, we discuss the rapid progress in perovskite-based photovoltaics and show results on Solaronix's novel "perovskite" solid-state mesoscopic solar cells.

Invited Talk TUT 5.4 Sun 17:55 HSZ 403

Perspectives of an artificial leaf based on inorganic semiconductors for water splitting: Device structure, interface engineering, catalytic demands — •Wolfram Jaegermann — TU Darmstadt, Instiute of Materials Science, Jovanka-Bontschits-Str. 2, D-64287 Darmstadt

For an effective conversion of solar energy to a chemical fuel a number of elementary processes as well as their coupling to each other must be optimized without severe losses in the number and the chemical potential of the originally generated electron-hole pairs. Light absorption coupled to efficient charge carrier generation and separation may be realized by thin film semiconductor devices - preferentially tandem cells - which may provide broad band quantum efficiencies close to 1. Alternatively, Janus type photocatalysts may be chosen which favour vectorial electron-hole pair transport into opposite directions. Subsequently, H2 (or HC-fuels) and O2 from H2O (and CO2) must be formed by electron and hole transfer reactions with minimized loss of chemical potential. This will only be possible if the involved charge transfer steps are coupled to selective multi electron transfer catalysts. Technologically feasible solutions seem to be possible for water splitting and H2-generation, as we will show with a number of investigations performed recently combining electrochemical investigations with surface science approaches.

Closing remarks