Working Group "Young DPG"
Arbeitskreis junge DPG (AKjDPG)

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Welcome to this year's programme of the Working Group "Young DPG"!

This year, three PhD Focus Sessions, organised by PhD students, present recent research areas to a broad audience. In addition, several participants present useful tools for the every day life of a physicists during our Hacky Hour.

You might wonder how to continue after your PhD?
A tutorial on Sunday as well as a lunch discussion on Thursday are presenting ways how to achieve success in academia. On the other hand, if you want to make your luck in industry, we offer in collaboration with the Working Group on Industrie and Business (AIW) lunch talks from Monday to Thursday presenting a different area every day where physicists are typically working. If you prefer to stay in the academic world, there is also a lunch session everyday in parallel covering various topics: DFG opportunities, Scientific Outreach, how to PostDoc and in collaboration with the Working Group on Physics, Modern IT and Artificial Intelligence (AKPIK) a lunch break with a follow up afternoon session will discuss the Nationale Forschungsdaten Infrastruktur (NFDI).

Beyond the scientific programme there will be our traditional Einstein Slam (in German) on Monday evening. If you want to get off the campus on Tuesday evening, then you are welcome to join our pub crawl to explore the Dresden night life.

We are looking forward to seeing you at our events!

Overview of Invited Talks and Sessions

(Lecture halls HSZ 02, HS 03, and HSZ 105)

Tutorial and Invited Talks

AKjDPG 1.1	Sun	16:00–16:45	HSZ 02	**Careers in science: "To boldly go where no one has gone before"** — •Manfred Fiebig
AKjDPG 6.1	Fri	9:30–10:00	HSZ 105	**Physicist in IT: Physics in Advent** — •André Wobst

Lunch Talks

PSV I	Mon	13:15–14:00	HSZ 03	**Wir sollten mal drüber reden (Physik und Wissenschaftskommunikation)** — •Axel Lorke, Nicolas Wöhrl
PSV II	Mon	13:15–13:45	HSZ 04	**Vom Physiker zum (erfolgreichen) Unternehmer der Plasway-Technologies GmbH** — •Stephan Wege
PSV III	Tue	13:15–14:00	HSZ 03	**Impact of the upcoming "Nationale Forschungsdaten Infrastruktur NFDI" on the SKM Community** — •Erich Runge, Cosima Schuster, Gert-Ludwig Ingold, Uwe Kahlert, Matthias Scheffler, Benjamin Wolba

PSV IV	Tue	13:15–13:45	HSZ 04	**Von der Physik zur Mode** — •Steve Kupke
PSV V	Wed	13:15–14:00	HSZ 03	**The German Research Foundation - Funding your Research** — •Ellen Reister, Michael Mössle
PSV VI	Wed	13:15–13:45	HSZ 04	**Thinking big in a small company, als Naturwissenschaftler in einem mittelständischen Familienunternehmen.** — •Jakob Bierwagen
PSV VII	Thu	13:15–14:00	HSZ 03	**How to "postdoc": Pathways after the PhD** — •Martin Wolf
PSV VIII	Thu	13:15–13:45	HSZ 04	**Working as a Physicist in Microelectronics** — •Matthias U. Lehr

Invited talks of the joint symposium SYCE

See SYCE for the full program of the symposium.

SYCE 1.1	Wed	9:30–10:00	HSZ 02	**Towards a carbon-free energy system: Expectations from R&D in renewable energy technologies** — •Bernd Rech, Rutger Schlatmann
SYCE 1.2	Wed	10:00–10:30	HSZ 02	**Decarbonizing the Heating Sector - Challenges and Solutions** — •Florian Weiser
SYCE 1.3	Wed	10:30–11:00	HSZ 02	**The challenge of anthropogenic climate change - Earth system analysis can guide climate mitigation policy** — •Matthias Hofmann
SYCE 1.4	Wed	11:15–11:45	HSZ 02	**A carbon-free Energy System in 2050: Modelling the Energy Transition** — •Christoph Kost, Philip Sterchele, Hans-Martin Henning
SYCE 1.5	Wed	11:45–12:15	HSZ 02	**The transition of the electricity system to 100% renewable energy: agent-based modeling of investment decisions under climate policies** — •Kristian Lindgren

Sessions

AKjDPG 1.1–1.1	Sun	16:00–17:15	HSZ 02	**Tutorial: Careers in Science (joint session AKjDPG/TUT)**
AKjDPG 2.1–2.9	Tue	9:30–13:00	HSZ 04	**PhD Focus Session: Symposium on "Strange Bedfellows – Magnetism Meets Superconductivity" (joint session MA/AKjDPG)**
AKjDPG 3	Tue	14:00–15:45	HSZ 03	**Envisioning Future Research Data Management (NFDI) from different Perspectives**
AKjDPG 4.1–4.4	Wed	15:00–17:15	HSZ 04	**PhD Focus Session: Symposium on "Magnetism – A Potential Platform for Big Data?" (joint session MA/AKjDPG/O)**
AKjDPG 5.1–5.4	Thu	17:15–18:30	ZEU 222	**PhD Focus Session: In-situ probes toward better understanding of hybrid halide perovskites I (joint session CPP/AKjDPG)**
AKjDPG 6.1–6.9	Fri	9:30–12:30	HSZ 105	**Hacky Hour**
AKjDPG 7.1–7.8	Fri	9:30–12:15	ZEU 222	**PhD Focus Session: In-situ probes toward better understanding of hybrid halide perovskites II (joint session CPP/AKjDPG)**

EinsteinSlam

Mon 20:00–21:30 HSZ 01

Pub Crawl

Tue 18:15 (after the ceremonial session) meeting point in front of HSZ

AKjDPG 1: Tutorial: Careers in Science (joint session AKjDPG/TUT)

Time: Sunday 16:00–17:15 Location: HSZ 02

Tutorial AKjDPG 1.1 Sun 16:00 HSZ 02
Careers in science: "To boldly go where no one has gone before" — •Manfred Fiebig — Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

What does it take to do a career in science and become a university professor? An obvious answer is: you have to do outstanding research. But just doing great science plays a surprisingly small part — and what defines ones scientific work as excellent anyway? Then, you also need to communicate your findings well. The best result is worth little if you present it in an awful talk or manuscript. You also need to be "good with people", may these be your students or your colleagues. Even luck can play an important role in asuccessful scientific career, but is very important to distinguish luck from "luck". I will refer to all these points and analyze what "being lucky" has actually to do with luck. I will present a list of points that I consider essential for a prosperous start into a scientific career. Some of these points are surprisingly unnoticed, so following them may put you ahead of the crowd.

Questions and discussion

AKjDPG 2: PhD Focus Session: Symposium on "Strange Bedfellows – Magnetism Meets Superconductivity" (joint session MA/AKjDPG)

At first sight, it seems that the phenomena of magnetism and superconductivity do not go along, as indicated by the Meissner effect, when a magnetic field is completely expelled from the interior of a conventional superconductor. However, the synergy of these two manifestations of nature in condensed matter does occur and can be rather interesting! Theoretical works have predicted the existence of exotic states at the interface between a superconductor and a magnet, such as the sought-after Majorana fermions and spin-triplet superconductivity. The first have been predicted to route an efficient way to implement quantum computers (currently a European scientific flagship), while the latter allows the creation of spin-polarized supercurrents, opening up fundamentally new possibilities for spintronics. Therefore, our symposium aims at putting together experts to provide a fundamental and practical understanding of the subject to discuss most recent developments from the theoretical and experimental sides, and to show perspectives for applications.

Organizers: Flaviano José dos Santos, Markus Hoffmann, Annika Stellhorn – (Forschungszentrum Jülich and Peter Grünberg Institut)

Time: Tuesday 9:30–13:00 Location: HSZ 04

Invited Talk AKjDPG 2.1 Tue 9:30 HSZ 04
Magnetism and superconductivity: building new physics one atom at a time — •Alexander Balatsky — Nordita and University of Connecticut

In this tutorial I will review the effects of magnetism and electronic defect in conventional and unconventional superconductors. The extreme case of quantum engineering where one builds magnetic and electronic features one atom at a time has proved to be a versatile approach. Impurities and defects are pair breakers in superconductors. I will discuss how defects can also enable new features in superconductors like intragap resonances, topological Majorana modes and seed new superconducting phases. Looking forward I will discuss how we might induce novel physics in superconductors with precise quantum impurity band engineering.

AKjDPG 2.2 Tue 10:15 HSZ 04
Magnetic Impurities and Anisotropic Multiband Superconductors — •Tom Saunderson[1], Gábor Csire[3], James Annett[1], Balázs Úfalussy[2], and Martin Gradhand[1] — [1]HH Wills Laboratory, University of Bristol, UK — [2]Wigner Research Centre for Physics, PO Box 49, H-1525 Budapest, Hungary — [3]Catalan Institute of Nanoscience and Nanotechnology (ICN2), Barcelona, Spain

Scanning tunnelling microscopy for superconductors has seen a flourish of activity in the last few years. It has become a powerful tool for determining the underlying fundamental properties of the gap structures in unconventional superconductors within the presence of impurities [1]. It has also been interesting to observe the pair-breaking effects that magnetic impurities have in conventional superconductors which lead to bound states [2]. Such states are even a possible source of Majorana Fermions [3]. We present the implementation of the Bogoliubov-de Gennes (BdG) equation into a Green's function (KKR) first principles method [4]. This method combines the full complexity of the underlying electronic structure and Fermi surface geometry with a simple phenomenological parametrisation for the superconductivity, whilst also being ideal to model impurities and interfaces. We present various test cases of simple superconductors in the presence of magnetic impurities, and assess the orbital character of the ensuing bound states.

[1] Ø. Fischer *et al*, Rev. Mod. Phys., **79**, 353 (2007)
[2] B. W. Heinrich *et al*, Prog. Surf. Sci., **93**, 1 (2018)
[3] S. Nadj-Perge *et al*, Science, **346**, 1259327 (2014)
[4] T. G. Saunderson *et al*, arXiv:1911.04163

Invited Talk AKjDPG 2.3 Tue 10:30 HSZ 04
Yu-Shiba-Rusinov states of single magnetic atoms and nanostructures probed by scanning tunneling spectroscopy — Eva Liebhaber[1], Michael Ruby[1], Benjamin W. Heinrich[1], Gaël Reecht[1], Kai Rossnagel[2,3], Felix von Oppen[1,4], and •Katharina J. Franke[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]Christian-Albrechts-Universität Kiel, Kiel, Germany — [3]Deutsches Elektronen Synchrotron, Hamburg, Germany — [4]Dahlem Center for Complex Quantum Systems, Berlin, Germany

The exchange coupling of individual magnetic atoms with the Cooper pairs of a superconducting substrate leads to Yu-Shiba-Rusinov (YSR) bound states inside the superconducting energy gap. Their bound state energy and spatial extent can be probed by scanning tunneling spectroscopy [1-4]. Chains of magnetic adatoms have attracted particularly strong attention due to the formation of Majorana bound states at their terminations [5].

Here, we investigate individual magnetic atoms on Pb and $2H$-$NbSe_2$ substrates. We observe intriguing patterns of YSR states around the adatoms, which are determined by the adatom's d-levels as well as local symmetries of the adsorption potential. When the adatoms are sufficiently close, the YSR states hybridize, eventually giving rise to YSR bands in atomic chains.

[1] Yazdani *et al.*, Science 275, 1767 (1997); [2] Ji *et al.*, Phys. Rev. Lett. 100, 226801 (2008); [3] Franke *et al.*, Science 332, 940 (2011); [4] Ménard *et al.*, Nature Phys. 11, 1013 (2015); [5] Nadj-Perge *et al.*, Science 346, 602 (2014).

AKjDPG 2.4 Tue 11:00 HSZ 04
Symmetric and antisymmetric combinations of Yu-Shiba-Rusinov states in antiferromagnetic dimers — •Philip Beck, Lucas Schneider, Levente Rósza, Jens Wiebe, and Roland

Wiesendanger — Department of Physics, University of Hamburg, Jungiusstraße 9-11, 20355 Hamburg

Magnetic atoms coupled to the Cooper pairs of a superconductor give rise to excitations in the superconductor's energy gap, so-called Yu-Shiba-Rusinov (YSR) states [1]. Theoretical proposals and experimental results have shown that, for ferromagnetically coupled atoms, the in-gap states hybridize and form symmetric and antisymmetric linear combinations.[2-4]

In our scanning tunneling spectroscopy study we reveal the evolution from multi-orbital YSR states of single transition metal atoms placed on an elemental superconductor to the YSR states of artificially constructed dimers with different interatomic separations and orientations. Even though the coupling in particular dimers, as calculated by DFT, is antiferromagnetic, we still observe a splitting of some of their orbital YSR states into symmetric and antisymmetric combinations. This unexpected behavior will be discussed and explained by advanced theoretical models.

We acknowledge funding by the ERC via the Advanced Grant ADMIRE (no. 786020) and by the SFB925 of the DFG.

[1] A. Rusinov, JETP **9**, 85 (1969). [2] D. K. Morr *et al.* PRB **67**, 020502 (2003). [3] M. Ruby *et al.* PRL **120**, 156803 (2018). [4] D.-J. Choi *et al.* PRL **120**, 167001 (2018).

Invited Talk AKjDPG 2.5 Tue 11:15 HSZ 04

Majorana bound states in magnetic skyrmions — •Jelena Klinovaja — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Magnetic skyrmions are highly mobile nanoscale topological spin textures. A magnetic skyrmion of an even azimuthal winding number placed in proximity to an s-wave superconductor hosts a zero-energy Majorana bound state in its core, when the exchange coupling between the itinerant electrons and the skyrmion is strong [1]. This Majorana bound state is stabilized by the presence of a spin-orbit interaction. We propose the use of a superconducting tri-junction to realize non-Abelian statistics of such Majorana bound states.

Antiferromagnetic skyrmion crystals are magnetic phases predicted to exist in antiferromagnets with Dzyaloshinskii-Moriya interactions. Their spatially periodic noncollinear magnetic texture gives rise to topological bulk magnon bands characterized by nonzero Chern numbers [2,3]. We find topologically-protected chiral magnonic edge states over a wide range of magnetic fields and Dzyaloshinskii-Moriya interaction values. Edge states appear at the lowest possible energies, namely, within the first bulk magnon gap. Thus, antiferromagnetic skyrmion crystals show great promise as novel platforms for topological magnonics.

[1] G. Yang, P. Stano, J. Klinovaja, and D. Loss, Phys. Rev. B 93, 224505 (2016). [2] S. Diaz, J. Klinovaja, and D. Loss, Phys. Rev. Lett. 122, 187203 (2019). [3] S. Diaz, T. Hirosawa, J. Klinovaja, and D. Loss, arXiv:1910.05214.

AKjDPG 2.6 Tue 11:45 HSZ 04

Interplay of Shiba and Majorana states in nanostructures deposited on superconducting surfaces — •Uriel A. Aceves-Rodriguez, Filipe S. M. Guimarães, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Majorana Bound States (MBS) are zero-energy modes that have become one of the leading candidates for the next generation of qubits, due to their topological protection and exchange statistics [1]. In pursuance of handling these entities, we implemented a multi-orbital tight-binding scheme, offering a realistic description of the electronic structure, to solve the Bogoliubov-de Gennes equations self-consistently. We investigate in-gap states, such as Shiba states, emerging from various nanostructures on typical superconducting substrates. Additionally, we examine the occurrence of MBS at superconducting/non-superconducting interfaces of nanowires deposited on superconducting surfaces.

This work was supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator Grant No. 681405-DYNASORE).

[1] J. Alicea, Rep. Prog. Phys. 75 (2012) 076501

Invited Talk AKjDPG 2.7 Tue 12:00 HSZ 04

Orbital selective superconductivity in iron-based superconductors — •Pengcheng Dai — Rice University

Superconductivity in iron-based superconductors emerges from long-range ordered antiferromagnetic phase with nematic order that breaks four-fold rotational symmetry of the underlying lattice. In spite of considerable work over the past decade, much is unclear concerning the microscopic origin of superconductivity and its relationship with magnetism, nematicity, and orbital order. In this talk, I will summarize our recent inelastic neutron scattering studies of iron-based superconductors, focusing on studying the relationship between magnetism, nematic order, and superconductivity. We find that orbital selective magnetic excitations and superconductivity are central to a microscopic understanding of these materials.

AKjDPG 2.8 Tue 12:30 HSZ 04

Inductive detection of field- and damping-like inverse spin-orbit torques in superconductor/ferromagnet heterostructures — •Manuel Müller[1,2], Lukas Liensberger[1,2], Luis Flacke[1,2], Hans Huebl[1,2,3], Akashdeep Kamra[4], Wolfgang Belzig[5], Rudolf Gross[1,2,3], Mathias Weiler[1,2], and Matthias Althammer[1,2] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), München, Germany — [4]Norwegian University of Science and Technology, Trondheim, Norway — [5]Fachbereich Physik, Universität Konstanz, Konstanz, Germany

Proximity effects at superconductor(SC)/ferromagnet(FM) interfaces provide novel functionality in the field of superconducting spintronics. We present experiments, where we probe the angular momentum transport across the SC/FM interface using a phase resolve broadband ferromagnetic resonance (bbFMR) technique that allows to measure both field- and damping-like inverse spin orbit torques (iSOT)[1]. We extend this iSOT analysis to make it applicable for SC/FM-bilayers and study iSOTs in a series of multilayers based on NbN/$Ni_{80}Fe_{20}$ as a function of temperature. We observe distinct changes in damping-like and field-like iSOT at the superconducting transition temperature T_c. Our findings reveal symmetry and strength of iSOTs at the SC/FM interface and provide guidance for future superconducting spintronics devices. [1] A. Berger. Phys. Rev. B. **97**: 94407. (2018).

AKjDPG 2.9 Tue 12:45 HSZ 04

Electronic and magnetic character of UTe_2 unconventional superconductor — Alexander B. Shick[1] and •Warren E. Pickett[2] — [1]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [2]Department of Physics, University of California-Davis, Davis, California, USA

The interplay between ferromagnetism and superconductivity is a challenging problem in the coupling between the two major states of condensed matter. We report density functional theory plus Hubbard U calculations for recently discovered the orthorhombic uranium dichalcogenide superconductor [1]. The UTe_2 displays superconductivity below 1.7 K, with the anomalous feature that the specific heat coefficient does not vanish at zero temperature limit, but rather weakly diverges, suggesting very low energy ungapped quantum fluctuations. The analysis of the experimental data indicates that this actinide compound is a nearly ferromagnetic spin-triplet superconductor. The DFT+U calculations for ferromagnetic alignment [2] reveal that the states are dominated by the j=5/2 configuration, with the $j_z = \pm 1/2$ sectors being effectively degenerate and half-filled. The Fermi surfaces are large and strongly metallic, and display low-dimensional features, reminiscent of the ferromagnetic superconductor UGe_2. Our calculations can provide a platform for modeling unusual behavior of UTe_2.

[1] S. Ran et al., Science 365, 684 (2019); [2] A. B. Shick, and W. E. Pickett, PRB 100, 134502 (2019).

AKjDPG 3: Envisioning Future Research Data Management (NFDI) from different Perspectives

Time: Tuesday 14:00–15:45 Location: HSZ 03

Bund und Länder haben im November 2018 den Aufbau einer Nationalen Forschungsdateninfrastruktur (NFDI) beschlossen. In der

NFDI sollen Datenbestände in einem aus der Wissenschaft getriebenen Prozess systematisch erschlossen, langfristig gesichert und entlang der FAIR-Prinzipien über Disziplinen- und Ländergrenzen hinaus zugänglich gemacht werden.
Im Rahmen der Session werden die einzelnen Aspekte des NFDI näher beleuchtet werden. Insbesondere wird es darum gehen, wie das Forschungsdatenmanagement in Zukunft aus verschiedenen Perspektiven aussehen könnte: Sowohl innerhalb der Physik z.B. für die Sektion Kondensierte Materie oder in der Teilchen- und Astrophysik, als auch darüber hinaus in der Chemie oder auch aus Sicht der jungen Physikerinnen und Physiker. Ziel ist es auch darüber ins Gespräch zu kommen, weshalb die Session nach fünf kurzen Vorträgen mit einer offenen Diskussion abschließen wird.
Diese Session schließt direkt an die Podiumsdiskussion PSV III an. Weitere Informationen zum Inhalt der Session finden sich im online Programm.

AKjDPG 4: PhD Focus Session: Symposium on "Magnetism – A Potential Platform for Big Data?" (joint session MA/AKjDPG/O)

As the title of a recent nature editorial article "Big data needs a hardware revolution" points out, new technologies and hardware architectures are necessary in order to cope with the ever increasing amount of information. Google's AlphaGo's success apprised of the potential of parallel computing, yet energy efficiency is a major challenge. Hardware developers came up with mimicking the human brain as the most efficient processor, leading to the field of neuromorphic computing. An immense amount of research is deployed in different fields to screen for fast, low energy consuming and scalable solutions. This focus session is meant to give insight into the current state-of-the-art computing together with its challenges as an introduction. Two major approaches to implement new computation technologies using magnetism, namely, neuromorphic computing based on spintronics, and wave-based computing using magnonics will be presented. A fourth talk, covering the prevailing use of magnetic tape for Big Data storage will give insight into the magnetic backbone of the largest information repositories.

Organizers: Mauricio Bejarano and Tobias Hula (Helmholtz-Zentrum Dresden Rossendorf), Luis Flacke and Lukas Liensberger (Walther-Meissner Institute and TU Munich)

Time: Wednesday 15:00–17:15 Location: HSZ 04

Invited Talk AKjDPG 4.1 Wed 15:00 HSZ 04
Data Storage and Processing in the Cognitive Era — •Giovanni Cherubini — IBM Research - Zurich

In this talk, I will present the emerging vision of cognitive data systems. A data system comprises physical devices that provide means to acquire, store and modify data for analytics and communications tasks, with the goal of obtaining high-value information. With the need to deal with exponentially growing amounts of data, however, the system size and complexity present major challenges for data storage and processing. In addition, with the approaching end of Moore's law, there is a dire need to significantly improve the efficiency of data systems in terms of cost and energy. To address these challenges, cognitive data systems will require novel learning algorithms and computing paradigms. The talk will be divided into two parts, focusing on data storage and processing aspects. First, I will present advanced technologies for big data storage systems, with focus on magnetic tape drives of future generations, targeting areal densities of several hundred gigabits per square inch on a flexible medium. Next, I will introduce in-memory computing techniques and devices that are well suited for novel computing systems, which are based on non-von Neumann architectures and aim at achieving the efficiency of the human brain.

Invited Talk AKjDPG 4.2 Wed 15:30 HSZ 04
Brain-inspired approaches and ultrafast magnetism for Green ICT — •Theo Rasing — Radboud University, Institute for Molecules and Materials, Heijendaalseweg 135, 6525AJ Nijmegen, the Netherlands

The explosive growth of digital data use and storage has led to an enormous rise in global energy consumption of Information and Communication Technology (ICT), which already stands at 7% of the world electricity consumption. New ICT technologies, such as Artificial Intelligence push this exponentially increasing energy requirement even more, though the underlying hardware paradigm is utterly inefficient: tasks like pattern recognition can be performed by the human brain with only 20W, while conventional (super)computers require 10 MW. Therefore, the development of radically new physical principles that combine energy-efficiency with high speeds and high densities is crucial for a sustainable future. One of those is the use of non-thermodynamic routes that promises orders of magnitude faster and more energy efficient manipulation of bits. Another one is neuromorphic computing, that is inspired by the notion that our brain uses a million times less energy than a supercomputer while, at least for some tasks, it even outperforms the latter. In this talk, I will discuss the state of the art in ultrafast manipulation of magnetic bits and present some first results to implement brain-inspired computing concepts in magnetic materials that operate close to these ultimate limits.

15 min. break.

Invited Talk AKjDPG 4.3 Wed 16:15 HSZ 04
How good are spin waves for data processing? — •Andrii Chumak — Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Vienna, Austria — Fachbereich Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany

Over the last decade, spin waves and their quanta magnons attract attention as data carriers in novel types of data processing units instead of electrons. Among the advantages proposed by spin waves, one can name added value given by the phase of the wave, pronounced nonlinear phenomena, scalability down to nm sizes, GHz to THz frequency range as well as low-loss information transport [1].

Recently, significant progress in the miniaturization of magnonic elements down to 50 nm took place [2, 3]. Moreover, a spin-wave directional coupler was investigated numerically [4] and realized experimentally on the nano-scale [5]. This is a universal unit allowing for the processing of analog RF and binary-coded digital information and is suitable for novel unconventional computing. E.g., the first integrated magnonic circuit in the form of half-adder was studied numerically [6].

Finally, now we are able to determine the parameters of future magnonic devices. The benchmarking of magnonic circuits with respect to 7 nm CMOS will be presented in the talk.

[1] A.V. Chumak, et al., Nat. Phys. 11, 453 (2015). [2] Q. Wang, B. Heinz, et al., Phys. Rev. Lett. 122, 247202 (2019). [3] B. Heinz, et al., arXiv: 1910.08801 (2019). [4] Q. Wang, P. Pirro, et al., Sci. Adv. 4, e1701517 (2018). [5] Q. Wang, M. Kewenig, et al., arXiv: 1902.02855 (2019). [6] Q. Wang, R. Verba, et al., arXiv: 1905.12353 (2019).

Invited Talk AKjDPG 4.4 Wed 16:45 HSZ 04
Unconventional computing with stochastic magnetic tunnel junctions — •Alice Mizrahi[1,2,3,4], Tifenn Hirtzlin[2], Matthew Daniels[3,4], Nicolas Locatelli[2], Akio Fukushima[5], Hit Kubota[5], Shinsi Yuasa[5], MD Stiles[4], Julie Grollier[1], and Damien Querlioz[2] — [1]Unité Mixte de Physique CNRS, Thales, Univ. Paris-

Sud, Université Paris-Saclay, 91767 Palaiseau, France — [2]Centre de Nanosciences et de Nanotechnologies, Univ. Paris-Sud, CNRS, Université Paris-Saclay, 91405, Orsay, France — [3]Maryland NanoCenter, University of Maryland, College Park, Maryland 20742, USA — [4]National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA — [5]Spintronics Research Center, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, 305-8568, Japan

Magnetic tunnel junctions are bi-stable nanodevices which magnetic state can be both read and written electrically. Their high endurance, reliability and CMOS-compatibility have made them flagship devices for novel forms of computing. While they are mostly used as non-volatile binary memories, they can be made unstable and thus behave as stochastic oscillators. Here, we show how stochastic magnetic tunnel junctions are promising elements for low energy implementations of unconventional computing. An analogy can be drawn between stochastic magnetic tunnel junctions and stochastic spiking neurons. We apply neuroscience computing paradigm to these devices and demonstrate that they can be the building blocks of low energy artificial neural networks capable of on-chip learning.

AKjDPG 5: PhD Focus Session: In-situ probes toward better understanding of hybrid halide perovskites I (joint session CPP/AKjDPG)

Metal-halide perovskites have attracted tremendous attention as absorber material in solar cells due to their rapid increase in power conversion efficiency. However, results within the field suffer from a range of variation and a lack of reproducibility. Thus detailed understanding of the highly dynamic material need correlation with the measurement conditions. To this end in-situ, operando and multimodal measurements are being developed. In this symposium, we want to bring together this in-situ expertise from various techniques which help to unravel material responses in hybrid perovskites. Organized by: Shambhavi Pratap (TU München), Hannah Funk (Helmholtz-Zentrum Berlin für Materialien und Energie) and Klara Suchan (Lund University, Sweden).

Time: Thursday 17:15–18:30 Location: ZEU 222

Invited Talk AKjDPG 5.1 Thu 17:15 ZEU 222

Real-time Investigation of Crystallization Pathways of Organo-Metal-Halide Perovskites Solar — •Michael F Toney — SLAC National Accelerator Laboratory, Menlo Park, Ca, USA

Perovskite solar cells (PSCs) have gained tremendous attention as materials for photovoltaics due to their high efficiencies and their compatibility with low-cost low-temperature fabrication methods (such as solution processing). Perovskite film formation is complex, involving the formation of intermediates and/or metastable phases that strongly affect the final perovskite film microstructure. Therefore, understanding the mechanism of perovskite formation and the crystallization pathways is key for facile control of perovskite formation. We are using time-resolved x-ray scattering to investigate the perovskite formation of MAPbI3-based perovskites and mixed cation (Cs, FA)PbI3 perovskites in-situ during spin coating and the subsequent post-deposition treatments. Our work highlights the importance of real-time investigation of perovskite film formation which can aid in establishing processing-microstructure-functionality relationships and help to provide a fundamental understanding of the mechanisms of perovskite formation.

AKjDPG 5.2 Thu 17:45 ZEU 222

Understanding the crystallization of solution processed, alloyed perovskites by multimodal characterization — •Shambhavi Pratap[1,2], Nobumichi Tamura[2], Zhenghao Yuan[3], Alastair MacDowell[2], Nicola Barchi[4], Jonathan Slack[2], Carolin Sutter-Fella[4], and Peter Müller-Buschbaum[1] — [1]Lehrstuhl für Funktionelle Materialien, TU München, 85748 Garching, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, 94720 Berkeley, USA — [3]Eberly College of Science, The Pennsylvania State University, State College,16801, USA — [4]Chemical Sciences Division, Lawrence Berkeley National Laboratory, 94720 Berkeley, USA

The crystallization behavior of solution processed hybrid plumbohalide perovskites is an ideal study to understand the formation of chemical alloys. Precursors corresponding to two different perovskites are mixed to serve as the precursor for an alloyed species. During crystallization, distinct crystalline species are isolated and characterized, as the equilibrium between the complex precursor intermediates and perovskites is transformed to the crystalline product by annealing the structure. The evolution of chemical structures is temporally resolved and the transient structures are studied for their optoelectronic transformation by photoluminescence.

AKjDPG 5.3 Thu 18:00 ZEU 222

Small-Footprint Optical Monitoring to Study Perovskite Thin Film Formation — Aboma Merdasa[1,2], Rahim Munir[1], Carolin Rehermann[1], Katrin Hirselandt[1], Janardan Dagar[1], Klara Suchan[2], and •Eva Unger[1,2] — [1]Helmholtz-Zentrum Berlin — [2]Lund University, Sweden

Record performance of Metal-Halide Perovskite (MHP) based solar cells have been achieved for small area devices based on spin-coating. Developing this device technology towards larger area prototypes will require the utilisation of scalable process technology. Processing strategies developed for spin-coating have been developed by incremental modifications of MHP ink and process conditions. Translating these processing strategies to scalable process technology requires a fundamental understanding of the formation mechanism. We recently developed a small-footprint spectroscopy setup based on fibre-optics enabling the monitoring of thin film formation processes. The setup can be easily integrated in process equipment such as spin-coater or slot-die coaters. UV-Vis measurements in reflectance mode enable us to describe the thinning of precursor solution during initial stages of MHP deposition as well as the onset of MHP crystallisation. As examples, the role of the anti-solvent drip in thin film formation, inhomogeneous crystallisation of MHP materials from mixed bromide/iodide precursors, crystallisation of reduced dimensional 2D/3D materials and effect of spin-coating and annealing time on MHP device performance will be discussed.

AKjDPG 5.4 Thu 18:15 ZEU 222

Investigating MAPbI_{3} Thin Film Formation during Spin Coating by Simultaneous in Situ Absorption and Photoluminescence Spectroscopy — Mihirsinh Chauhan[1,2], Yu Zhon[1], Konstantin Schötz[1], Brijesh Tripathi[2], Anna Köhler[1], Sven Huettner[1], and •Fabian Panzer[1] — [1]University of Bayreuth, Bayreuth, Germany — [2]Pandit Deendayal Petroleum University, Gandhinagar, India

Until today, the two-step processing method represents an attractive route for the thin film formation of halide perovskites. However, a fundamental understanding about the film formation dynamics in case of spin coating methylammonium iodide (MAI) on PbI_{2} has not been established yet. Here we apply in-situ optical spectroscopy during the two-step film formation of the model halide perovskite MAPbI_{3} via spin coating. We identify and analyze in detail the optical features that occur in photoluminescence and corresponding absorption spectra during processing. We find that the film formation takes place in five consecutive steps, including the formation of a MAPbI3 capping layer via an interface crystallization and the occurrence of an intense dissolution-recrystallization process. Consideration of confinement and self-absorption effects in the PL spectra, together with consideration of the corresponding absorption spectra allows to quantify the growth rate of the initial interface crystallization to be 13 nm/s for our processing conditions. We find the main dissolution recrystallization process to happen with a rate of 445 nm/s, emphasizing its importance to the overall processing.

AKjDPG 6: Hacky Hour

Time: Friday 9:30–12:30 Location: HSZ 105

Invited Talk AKjDPG 6.1 Fri 9:30 HSZ 105

Physicist in IT: Physics in Advent — •André Wobst — wobsta GmbH, Unterschleißheim

For more than 17 years I am working as a service provider in planning, realization and administration of physics-related IT projects. Here I present one of the projects, namely a physics Advent calendar. The technology stack is rather common and efficient: Python, Flask, PostgreSQL to name just the most important building blocks. The load of such a project (more than 43,000 users in 2019, all within a few weeks and with high daily return rate) is operated on moderate infrastructure by taking into account efficiency right from the start. I overview challenges that arise during implementation and operation and show some web analytics, monitoring data and report on attacks. I will also discuss a few pitfalls like avoiding backpressure (a term adopted from fluid dynamics to IT).

AKjDPG 6.2 Fri 10:00 HSZ 105

Reproducible workflows for reproducible science (with Snakemake) — •Johannes Hampp — Center for international Development and Environmental Research, Justus Liebig University Giessen

Daily scientific tasks with research data from experiments or simulations often imply repetitively applying the same analysis steps. Be it with R, Python or other programming languages, analysis workflows too often followed by hand. Executing analysis steps manually be the obvious approach, but is tedious and prone to human error. In this talk I introduce you to Snakemake, an open source solution for managing your workflows. Snakemake allows for well-defined workflows, with steps executed automatically in the correct and necessary order. It decreases the amount of non-scientific work spent in repetetive workflows and reduces unecessary errors. Since workflows are defined in a simple and human-readable format, using Snakemake helps to document your analysis. It increases reproducibility of research and lastly the FAIRness of research data.

In short: Snakemake makes your life a lot more fun.

AKjDPG 6.3 Fri 10:15 HSZ 105

How to Optimize your Productivity using Tiling: Terminal Multiplexing with `tmux` and Window Managing with `i3` — •Mario Udo Gaimann — Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, Germany

In this talk I will introduce you to two useful tools that can improve your workflow. In essence, they both offer a keyboard-controlled management of your workspaces and terminals which may – with some practise – boost your efficiency.

Firstly, I will introduce you to the terminal multiplexer `tmux`, a versatile tool to enhance your command line productivity. You will learn how to create, detach and attach `tmux` sessions and how to split your terminal into multiple panes and windows.

Secondly, we will have a look at the window manager `i3`, a desktop environment that allows you to optimize your workspace organization. Here you will learn how to open terminals and applications in an `i3` environment, create and split windows, change container layouts, and create new workspaces.

AKjDPG 6.4 Fri 10:30 HSZ 105

Better than histograms: Kernel density estimators and why you should use them — Alexandra Völkel[1] and •Simeon Völkel[2] — [1]Universität Bayreuth, Experimentalphysik VIII, Universitätsstraße 30, 95447 Bayreuth, Germany — [2]Universität Bayreuth, Experimentalphysik V, Universitätsstraße 30, 95447 Bayreuth, Germany

We show why everyone who has ever made a histogram should learn about kernel density estimation.

Histograms, as commonly used for estimating probability densities, are far from being optimal. In addition, they require two parameters, bin width and position, to be chosen.

Kernel density estimators are an easy to use drop-in replacement for virtually all histograms you ever wanted to draw. They combine superior mathematical properties with an at least as intuitive presentation. Their bandwidth, being the only parameter, can be chosen in an optimal sense automatically and adaptively.

Regarding practical application, we discuss their usage in gnuplot and python.

AKjDPG 6.5 Fri 10:45 HSZ 105

LeMonADE - A Lattice Monte Carlo Library — •Martin Wengenmayr[1,2], Toni Müller[1,2], and Ron Dockhorn[1] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]TU Dresden, Germany

LeMonADE is a **L**attice-based **e**xtensible **Mon**te-Carlo **A**lgorithm and **D**evelopment **E**nvironment library developed in the group “Theoretical Polymer Physics” of the Leibniz Institute for Polymer Research. It provides a C++ template meta programming interface for Monte Carlo simulations specialized for the Bond Fluctuation Model to investigate polymeric materials. Based on compile-time generated code, the framework provides containers for coordinates, topologies, and various types of metadata, also basic evaluation tools and convenience methods for I/O file handling using a human readable, compressed file format. LeMonADE has been used to simulate a wide variety of coarse-grained polymer systems under excluded volume conditions, selective solvents, nearest neighbor interactions, polymerization processes, external potentials, and even more. In addition to the CPU-based library some GPU accelerated modules are available benefiting from multiprocessor architectures. Furthermore, a visualization tool is offered as well. The project is hosted under GPL on github [https://github.com/LeMonADE-project] with a continuous integration framework running a large set of unit tests. The library has already been used for a wide range of research topics and for several publications in the field of theoretical polymer science.

AKjDPG 6.6 Fri 11:00 HSZ 105

`pyscal`: A python module for structural analysis of atomic environments — •Sarath Menon, Grisell Díaz Leines, and Jutta Rogal — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, Germany

Structural characterisation of local atomic environments is essential to provide insight into atomistic mechanisms of transformations between crystalline and liquid phases, or the formation and dynamics of extended defects that govern materials properties. The development of methods and tools to analyse the local structure constitutes a central step in the evaluation of atomistic simulation data. `pyscal` is a Python module designed for the computation of local structural order parameters during post-processing of atomistic trajectories. `pyscal` provides various approaches for structural characterisation such as Steinhardt's bond order parameters, tools for Voronoi tessellation, algorithms for clustering of atoms, and additional structural features such as radial distribution function and coordination numbers. While Python offers the advantage of flexibility and extensibility, the core code for `pyscal` is written in C++ to ensure fast and efficient calculations. `pyscal` brings together various methods for structural analysis in a single module, making it a useful tool for analysis and for applications such as feature engineering for machine learning. The source code for pyscal is available from the repository(`https://github.com/srmnitc/pyscal`) and documentation including examples are available on pyscal website(`https://pyscal.com`).

AKjDPG 6.7 Fri 11:15 HSZ 105

Scaling of Hybrid Quantum Classical Annealing — •Aditi Misra-Spieldenner[1], Peter Ken Schuhmacher[1], Xi Dai[2], Salil Bedkihal[2], and Frank K Wilhelm[1] — [1]Universität des Saarlandes — [2]University of Waterloo

In an earlier work an efficient gap-independent cooling scheme has been proposed for a quantum annealer that benefits from finite temperatures for single qubit systems based on superconducting flux qubit [1]. In our current work we extend this investigation to systems containing larger number of qubits. We simulate random annealing schedules using a well established path integral method called 'Quasi Adiabatic Propagator Path Integral' (QUAPI). We investigate different cooling methods to counter noise and heating that arise from always present longitudinal thermal noise.

[1]'Gap-independent cooling and hybrid quantum-classical annealing', L. S. Theis, Peter K. Schuhmacher, M. Marthaler, F. K. Wilhelm

AKjDPG 6.8 Fri 11:30 HSZ 105

LEED Analysis Software: LEEDCal and LEEDLab — •Roman Forker, Felix Otto, Falko Sojka, and Torsten Fritz — Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena (Germany)

Low-energy electron diffraction (LEED) can be used to measure surface lattice parameters very accurately, under the condition that the device is properly calibrated. LEEDCal provides a powerful algorithm to determine and correct systematic distortions in LEED images. Easy to operate via its graphical user interface, LEEDCal automatically generates a correction matrix upon analyzing a reference sample exhibiting a well-known surface structure. This matrix can be applied to rectify all future diffraction patterns recorded with the same LEED device. This also works in batch mode.

The results allow interpreting accurately and objectively the lattice constants and epitaxial relations when used in combination with LEEDLab, a software package that simulates LEED patterns and analyzes them quantitatively.

In our contribution, we demonstrate the functionality of the LEED analysis software packages LEEDCal and LEEDLab by means of an instructive example.

https://www.organics.uni-jena.de/en/Research.html

AKjDPG 6.9 Fri 11:45 HSZ 105

Characterizing the speed, size and shape of droplets during their flight from an ultrasonic spray coater — •Pieter Verding — Uhasselt, Hasselt, Belgium

Ultrasonic spray coating is a technology offering many new possibilities, such as depositing ultrathin homogeneous layers up to 20 nm on large scale. However, its industrial application is limited due to many process parameters which have a large impact on the quality of the coating. For this reason, measuring the droplet size, speed, and concentration during the flight from the ultrasonically generated droplet to the substrate, will give insight in how to tune the process parameters. For inkjet printing, this led to dimensionless numbers that perfectly describe the ink formulation suitable for printing. However, inkjet printing is jetting only one droplet at the time, where for ultrasonic spray coating, thousands of droplets are created at the same time, making measuring the properties of the droplets during flight a complicated task.

Three different measurement techniques (Dynamic Light Scattering, Turbidimetry and a High Speed Camera as reference) have been developed in and around an ultrasonic spray coating setup. Dynamic Light Scattering shows, after Fourier transformation, shifted peaks, representing the speed of the droplets. Further, applying Turbidimetry, it is possible to determine the size of the droplets from the speed as defined by Dynamic Light Scattering. Droplets size and speed could be measured and gave comparable results as measured with a High Speed Camera. Further, the influence of the process parameters

Discussions and Tool testing

AKjDPG 7: PhD Focus Session: In-situ probes toward better understanding of hybrid halide perovskites II (joint session CPP/AKjDPG)

Time: Friday 9:30–12:15 Location: ZEU 222

Invited Talk AKjDPG 7.1 Fri 9:30 ZEU 222

Time-resolved X-ray scattering to understand perovskite materials — Oliver Filonik[1], Christopher Greve[2], Meike Kuhn[2], Michael Buchhorn[2], Adrian Ebert[2], Richard Kellnberger[2], and •Eva M. Herzig[1] — [1]MSE - Herzig Group, TU München, Lichtenbergstr. 4a, 85748 Garching — [2]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth

The formation of perovskite thin films is of interest since this process determines the final material quality. In-situ X-ray scattering can help to learn more about the formation of perovskite crystals and how the crystallization is altered by the use of additives or other parameters. The film formation mechanism directly influences the performance of, for example, solar cells. We apply different techniques to extract time-resolved information and will show the opportunities and limitations of these in the quest for understanding formation-function relationships in perovskites.

AKjDPG 7.2 Fri 10:00 ZEU 222

In situ reflectometry and air flow control enables modeling of the drying process in blade coated hybrid perovskite solution films. — •Simon Ternes[1,2,3], Tobias Börnhorst[3], Jonas A. Schwenzer[1], Ihteaz M. Hossain[1,2], Uli Lemmer[1], Philip Scharfer[2,3], Wilhelm Schabel[3], Bryce S. Richards[1,2], and Ulrich W. Paetzold[1,2] — [1]Light Technology Institute, Karlsruhe, Germany — [2]Institute of Microstructure Technology, Eggenstein-Leopoldshafen, Germany — [3]Institute of Thermal Process Engineering, Karlsruhe, Germany

In recent years, hybrid perovskite solar cells (PCSs) have been introduced to the field of thin-film photovoltaics, exhibiting not only a steep increase in power conversion efficiencies from 3.8% in 2009 to above 25% to date, but also opening the perspective toward low-cost, large-scale solution processing. However, in order to design industrial-scale printing machines for PCSs in an efficient manner, general modeling of the dynamic drying and crystallization processes in perovskite solution films is required. This modeling must extend beyond trail-and-error optimization and beyond the commonly used, non-scalable spin coating technique. In the work presented here, we demonstrate simultaneous exact drying control by a laminar air flow and in situ film thickness measurements by reflectometry on blade coated perovskite solution films. In this way, we derive a general model of the drying process in these solution films and correlate it with the evolving morphology, providing a strategy of optimal process transfer from spin coating to any industrial coating and drying technique.

AKjDPG 7.3 Fri 10:15 ZEU 222

The zero step for degrading perovskite solar cells: what atmosphere should we choose? — •Renjun Guo[1], Wei Chen[1], Lennart K. Reb[1], Manuel A. Scheel[1], Stephan Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]Deutsches Elektronen-Synchrotron (DESY), Notkestrasse 85, 22607 Hamburg, Germany

The power conversion efficiency (PCE) of perovskite solar cells (PSCs) reached the champion value of 25.2 percent, making this technique competitive with commercial silicon solar cells. Despite such advantages, the application of PSCs is currently limited by combining high performance and operational stability because PCE of PSCs can degrade due to the presence of temperature, light, humidity, and oxygen. Besides, current degradation research on PSCs is carried out without standard protocol. Therefore, it is necessary to make the standard protocol for the long term degradation of PSCs. We investigated degradation processes of PSCs under both AM 1.5G and different atmosphere conditions with in-situ grazing incidence wide-angle X-ray scattering (GIWAXS) and grazing incidence small-angle X-ray scattering (GISAXS). With these approaches, we can follow the evolution of characteristic structures and of the inner morphology under the operational condition. After understanding the degradation mechanisms upon different atmosphere (nitrogen and vacuum), we can choose a reasonable atmosphere which allows for the standard aging routine to guide industrial development.

AKjDPG 7.4 Fri 10:30 ZEU 222

Growth of Methylammonium and Formamidinium Lead Halides by Co-Evaporation Analyzed with in situ X-ray Diffraction — •Karl Heinze, Thomas Burwig, Roland Scheer, and Paul Pistor — Martin-Luther-Universität Halle-Wittenberg, Halle an der Saale, Germany

Crystalline lead halide perovskite (e.g. Methyl Ammonium (MA) PbI_3), thin-film solar cells reach efficiencies far over 20%. These films are commonly prepared by solvent-based methods such as spin-coating, with limited scalability. An industrially attractive technique for the deposition of thin films is co-evaporation. Using a vacuum chamber with a built-in in-situ X-ray diffraction system, we are able to investigate the influence of varying processing conditions during the co-evaporation of MA lead halides ($MAPbX_3$, with X=I,Br,Cl) and formamidinium lead halides ($FAPbX_3$) on the film formation process and can cross-relate our findings to opto-electronic properties and solar cell performance. More specifically, we analyze the effect of different precursors flux rate ratios and substrate temperatures on the crystal growth and compare sequential to simultaneous co-evaporation. We find a strong impact of the processing temperature on crystal size and morphology and determine suitable process windows for optimal absorber compositions with small amounts of PbI_2 secondary phases. We note that processing conditions have also a strong impact on the crystal orientation of the films. This is especially pronounced for $FAPbBr_3$, where we were able to grow films with nearly complete orientation in either (100) or (111) direction.

Invited Talk AKjDPG 7.5 Fri 10:45 ZEU 222

Structural dynamics of halide perovskites via in-situ electron microscopy — •Chen Li — Electron microscopy for Materials research (EMAT), University of Antwerp, Antwerp, Belgium

In-situ microscopy is a powerful tool to investigate dynamic transformations in materials. To observe such transformations the focused electron probe in scanning transmission electron microscope (STEM) can be used to both stimulate and image the movement of atoms [1]. Here we apply such dynamic STEM to directly observe ion migration in hybrid and inorganic halide perovskites.

Direct in-situ heating of samples can also be used inside electron microscopes to provoke phase changes with special heating holders [2]. We use in-situ heating in STEM to track the phase transitions in inorganic CsPbI3 perovskites from an orthorhombic δ- phase to a cubic α-phase. An intermediate phase with layered configuration was observed during the transition.

[1] C. Li, Y. Y. Zhang, T. J. Pennycook, Y. L. Wu, A. R. Lupini, N. R. Paudel, S. T. Pantelides, Y. Yan and S. J. Pennycook, Column-by-column observation of dislocation motion in CdTe: dynamic scanning transmission electron microscopy, Appl. Phys. Lett. 2016, 109, 143107

[2] C. Li, E. S. Sanli, H. Strange, M. D. Heinemann, D. Greiner, R. Mainz, W. Sigle, D. Abou-Ras and P. A. v. Aken, Diffusion-assisted grain boundary migration in CuInSe2. under review

15 min. break

AKjDPG 7.6 Fri 11:30 ZEU 222

Band structure and electronic properties of lead halide perovskites from photoemission studies — •Fengshuo Zu[1,2], Patrick Amsalem[1], David Egger[3], Christian Wolff[4], Rongbin Wang[1,7], Maryline Ralaiarisoa[1], Honghua Fang[5], Maria Antonietta[5], Dieter Neher[4], Leeor Kronik[6], Steffen Duhm[7], and Norbert Koch[1,2] — [1]HU Berlin — [2]HZB Berlin — [3]TU Munich — [4]Universität Potsdam — [5]University of Groningen, Netherland — [6]Weizmann Institute of Science, Israel — [7]Soochow University,China

Photovoltaic devices based on halide perovskites with outstanding optoelectronic properties have exhibited tremendous progress in performance. To understand the origin of these properties comprehensively, detailed knowledge on the underlying electronic band structure is required. Here, we present complementary results from low-energy electron diffraction, angle-resolved photoelectron spectroscopy, and density functional theory calculations for CH3NH3PbBr3 and CH3NH3PbI3 single crystals. For both, sharp LEED patterns corresponding to the (001) surfaces of CH3NH3PbBr3 and CH3NH3PbI3 were observed together with well-resolved, dispersive valence band features. Furthermore, the fundamental differences between linear and logarithmic methods in determining the VB onset are discussed and addressed.[1] In addition, surface photovoltage effect, which has so far hardly been discussed in this context, is found to play significant effect in photoemission studies.[2] [1] Zu et al., J. Phys. Chem. Lett. 2019, 10, 601,[2] Zu et al., ACS Appl. Mater. Interfaces, 10.1021/acsami.9b05293.

AKjDPG 7.7 Fri 11:45 ZEU 222

Energy-Level Alignment of Formamidinium Tin Iodide with Organic Contact Materials — •Jonas Horn, Pascal Schweitzer, and Derck Schlettwein — Justus Liebig University Gießen, Institute of Applied Physics

The alignment of energy levels at the interfaces of a perovskite absorber with adjacent hole- and electron-transporting materials affects the formation of space-charge regions and interfacial recombination. These have consequences for charge transport in the layers and for the efficiency of devices. To analyze such alignment we used Kelvin-probe force microscopy (KPFM). This study is focused on formamidinium tin iodide ($FASnI_3$) as perovskite absorber, which avoids the toxicity problems of lead and is known to yield the highest power conversion efficiencies amongst all lead-free perovskite absorbers. The most common solar cell geometry for $FASnI_3$ implements C_{60} as electron-transporting material, which is prepared onto the perovskite by physical vapor deposition (PVD). Intermittently to PVD, we used KPFM to simultaneously monitor morphology and work function of C_{60} during its growth on $FASnI_3$. We show that a sufficiently high deposition rate is needed to avoid island formation of C_{60} and obtain a homogeneously covering film with constant work function. We further show that the width of the space charge layer in C_{60} is larger than the film thickness often implemented in perovskite solar cells. A band bending in the range of 300 meV is observed and consequences for prospective device operation are discussed.

AKjDPG 7.8 Fri 12:00 ZEU 222

Thermal decomposition dynamics of lead halide perovskite thin films — Thomas Burwig, Karl Heinze, Roland Scheer, and •Paul Pistor — MLU Martin-Luther-Universität Halle-Wittenberg

Despite the remarkable progress of lead halide perovskites, their low stability severely limits practical applications. To understand degradation pathways and pinpoint optimal compositions in terms of stability is therefore of utmost importance. Here we investigate the thermal stability of lead halide perovskite thin films grown by co-evaporation and analyze their thermal decomposition at elevated temperatures. Our approach allows to investigate the thermal decomposition by time-resolved in situ X-ray diffraction inside the vacuum growth chamber, without exposing the perovskite thin film to moisture or ambient air at any time. By applying fixed temperature ramps of 3-4 K/min. , we compare the onset of decomposition for a variety of different ABX_3 compositions and explore perovskites throughout the compositional space with A=MA,FA,Cs; B=Pb,Sn,(Ag,Bi) and X=I,Br,Cl. We find an increasing decomposition temperature for the series $MAPbCl_3$ - $MAPbI_3$ - $MAPbBr_3$, where the perovskite decomposes via degassing of MAX. The cation variation shows increased stability for $CsPbBr_3$ over $FAPbBr_3$ and $MAPbBr_3$, mainly due to the increased sublimation temperature of CsX, which is even higher than that of PbX_2. Finally, for the case of the most common and less stable $MAPbX_3$ perovskites, a series of time-resolved degradation experiments at constant temperatures provides detailed insights into the degradation kinetics of these materials.