Working Group on Physics, Modern IT and Artificial Intelligence Arbeitskreis Physik, moderne Informationstechnologie und Künstliche Intelligenz (AKPIK)

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Overview of Invited Talks and Sessions

(Lecture hall HSZ 301; Poster P2/1OG)

Sessions

AKPIK 1.1–1.8	Mon	16:45–18:45	HSZ 301	**AKPIK Talks**
AKPIK 2.1–2.4	Mon	18:45–19:30	P2/1OG	**AKPIK Posters**

AKPIK 1: AKPIK Talks

Time: Monday 16:45–18:45 Location: HSZ 301

AKPIK 1.1 Mon 16:45 HSZ 301

Insights of a statistical analysis of Cu/SiO2/W devices for memory applications — •Florian Maudet[1], Veeresh Deshpande[1], Hanno Kröncke[1], and Catherine Dubourdieu[1,2] — [1]Institute Functional Oxides for Energy-Efficient Information Technology (EM-IFOX), Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Freie Universitat Berlin, Physical Chemistry, Arnimallee 22, 14195 Berlin Germany

Resistance switching memories are promising candidates for low power consumption non-volatile memory applications owing to their dimensional scalability and fast switching speed. Among the proposed systems, Cu/SiO2 based memory devices have demonstrated very promising performances and allow easy integration with CMOS technology. In such systems the different states originate from the formation of a Cu filament in the SiO2 solid electrolyte. Because of this, the devices are very sensitive to local inhomogeneities like defects in the SiO2 dielectric or interface roughness. As a result, the on/off resistance and the set/reset voltage can have significant device-to-device variations limiting their advantages for potential applications. In order to quantify and understand the origin of the distribution of these characteristics we present a broad statistical analysis of Cu/SiO2/W memory behavior. The influence of different voltage sweep rates and device areas are investigated. This study allows identification of key parameters that can be optimized to reduce variance between samples.

AKPIK 1.2 Mon 17:00 HSZ 301

Fast fitting of reflectivity data of growing thin films using neural networks — •Alessandro Greco[1], Vladimir Starostin[1], Christos Karapanagiotis[2], Alexander Hinderhofer[1], Alexander Gerlach[1], Linus Pithan[3], Sascha Liehr[4], Frank Schreiber[1], and Stefan Kowarik[4] — [1]Institut für Angewandte Physik, University of Tübingen, Auf der Morgenstelle 10, Tübingen 72076, Germany — [2]Institut für Physik, Humboldt Universität zu Berlin, Newtonstrasse 15, Berlin 12489, Germany — [3]European Synchrotron Radiation Facility, 71 Avenue des Martyrs, Grenoble 38000, France — [4]Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, Berlin 12205, Germany

X-ray reflectometry is a powerful and popular scattering technique that can give valuable insight into the structure and growth behavior of thin films. This study [1] shows how a simple artificial neural network model can be used to determine the thickness, roughness and electron density of thin films of different organic semiconductors [diindenoperylene, copper(II) phthalocyanine and α-sexithiophene] on SiO_2 from their reflectivity data with millisecond computation time and with minimal user input or *a priori* knowledge. For a large experimental data set of 372 XRR curves, it is shown that a simple fully connected model can provide good results with a mean absolute percentage error of 8–18% when compared with the results obtained by a genetic least mean squares fit using the classical Parratt formalism. Furthermore, current drawbacks and prospects for improvement are discussed.

[1] Greco et al., *J. Appl. Cryst.* (2019). **52**, 1342–1347

AKPIK 1.3 Mon 17:15 HSZ 301

Detecting noise-blurred deterministic signals with neural networks trained with synthetic data — •Lazaro Alonso Silva, Alexander Eisfeld, Sebastian Gemsheim, and Jan Michael Rost — Max-Planck-Institut für Physik komplexer Systeme, Dresden Germany

We investigate the transferability of artificial neural networks trained on synthetic data with characteristic pattern and noise added to real data to extract the underlying pattern. This is useful when the generation of real training data is computationally expensive or scarce. Using synthetic data from an ideal periodic signal with noise added, we analyse how the extraction capability for a given noise level depends on the size of the training data and the architecture and complexity of the network. We find that networks are most robust in recognizing the periodic signal in noisy data if trained with ideal periodic signals including an optimal amount of noise dependent on the size of the training data. Applied to atomic high harmonic spectra, which are naturally noisy, we can extract their periodicity. In addition, the scheme described allows us to estimate the noise level in the high harmonics spectra.

AKPIK 1.4 Mon 17:30 HSZ 301

Artificial Intelligence for the discovery of new molecules — •James Nelson and Stefano Sanvito — Trinity College Dublin, Dublin, Ireland

Many problems facing society today have their solution partially in the discovery of new molecules and materials, i.e. designing energy-efficient technology and drug discovery. However, the space of possible materials is enormous and the known set of compounds only scratches the surface. We propose to use Generative Adversarial Networks (GANs) to help explore this chemical space and suggest new potential compounds. Here we have two neural networks, with one network suggesting potential molecules and another acting as a critic. The two networks compete against each other, resulting in the generative network being able to produce realistic molecules.

In this talk, I'll show our preliminary results in applying GANs to molecules. In particular, we have: designed a unique GAN that incorporates structural information, been able to reproduce thermal distributions of a diverse set of molecules and found chemically sound molecules and that maximise some criteria. This work paves the way towards the use of Artifical Intelligence as a tool to search through chemical space.

AKPIK 1.5 Mon 17:45 HSZ 301

Unsupervised phase discovery with deep anomaly detection — •Korbinian Kottmann[1], Patrick Hümbeli[1], Maciej Lewenstein[1,2], and Antonio Acín[1,2] — [1]ICFO, Avinguda Carl Friedrich Gauss, 3, 08860 Castelldefels — [2]ICREA, Passeig de Lluís Companys, 23, 08010 Barcelona

We present a novel method for automated and unsupervised discovery of new and unknown phases in quantum many-body scenarios. Instead of supervised learning, where data is classified using labeled data, we perform anomaly detection, where the task is to differentiate a normal data set, composed of one or several classes, from anomalous data. We propose a scheme, employing deep neural networks, to map out the whole phase diagram. The method can be used completely unsupervised and automated to explore the entire phase diagram. As a paradigmatic example, we explore the phase diagram of the extended Bose Hubbard model in one dimension at integer filling. We compute the ground states using tensor networks and exemplarily use both unprocessed data like the central tensor and processed data like entanglement spectra that suffice to reproduce the phase diagram. The formulation of the method is independent of the nature of the data and could as well be used with physical observables, i.e. experimental data.

AKPIK 1.6 Mon 18:00 HSZ 301

Machine Learning the Physical Non-Local Exchange-Correlation Functional of Density-Functional Theory — •Jonathan Schmidt, Carlos Benavides-Riveros, and Miguel Alexandre Lopes Marques — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle (Saale), Germany

We train a neural network as the universal exchange-correlation functional of density-functional theory to reproduce both the exact exchange-correlation energy and the exchange-correlation potential. By using the automatic differentiation functionality present in modern machine-learning frameworks, we impose the exact mathematical relation between the exchange-correlation energy and the potential, leading to a fully consistent method. The developed functional is extremely non-local, but retains the computational scaling of traditional local or semi-local approximations. It therefore holds the promise of solving some of the delocalization problems that plague density-functional theory, while maintaining the computational efficiency that characterizes the Kohn-Sham equations. We demonstrate the feasibility of our approach by looking at strongly-correlated one-dimensional electronic systems, where density-functional methods are known to fail, and investigate the behavior and performance of our functional by varying the degree of non-locality.

AKPIK 1.7 Mon 18:15 HSZ 301

Wat is Artificial Intelligence? — •Norbert Sadler — Wasserburger Str. 25a 85540 Haar

Current AI processses are used for pattern-based analyses of big data,

which in turn enable autonomous decision making. AI is not being integrated or expanded into scientific decision making based on nature constants and physical laws.

We are looking for a "human Interface" linked to AI as well as to the synchronously firing eigenvalue frequency of the innovative alpha- and beta waves in the relaxed part of the brain at a frequency range of 8-16 Hz.

AI can access the alpha-and beta waves based on a linear mapping of the Josephson frequency f(J)=2x(0.1eV)/(h). This can occur at a neuronal potential of 0.1 Volt, from the overlaid quantum state to the 10**11 neurons and the 10**14 synapses of the brain. The linear mapping follows Heisenberg's matrix mechanics.

f(J)=2x(0.1eV)/(h)=2x(15.6 X 15.6)Hz x 10**11 neurons/brain.

f(J)=2x((1/64 Codons) X 15.6)Hz x 10**14 synapses/Neuron. The Josephson frequency f(J)=15.6 Hz is associated with the brain waves!. For further AI-associated Interfaces can be found:. On cosmolology: f(AI)=(69% dark E.)/(4.5% bar. Mat.)=15.3. On the entropy: f(AI)=1/(entropy 0.066)=e**e=15.15. On the golden ratio Phi: f(AI)=3Pi x Phi(1.618)=15.3. Conclusion: AI is a fraktal of the neurological intelligence and applicable in science and technique. Information: www.artificial-intelligence-in-science.com

AKPIK 1.8 Mon 18:30 HSZ 301

Quantum-computer calculations of the ground state energy of negative hydrogen ion — •Ivana Miháliková[1,2], Martin Friák[1,2], Matej Pivoluska[3], Martin Plesch[3], and Mojmír Šob[4,1,5] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Brno, Czech Republic — [3]Institute of Computer Science, Masaryk University, Brno, Czech Republic — [4]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [5]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

Quantum computing has become one of the most popular applications of quantum physics. Importantly, it is believed that quantum computers will surpass the efficiency of classical computers in near future. A wide range of problems in condensed matter physics and chemistry could be solved by quantum computers. Nowadays, IBM provides a cloud-based quantum computing platform (IBM Quantum Experience) offering five-qubit and sixteen-qubit quantum processors for a real run. In our study, we focused on the quantum simulation of negative hydrogen ion. We perform the simulations of the H^- ground state energy using Variational Quantum Eigensolver (VQE). Simulations were performed on the QASM simulator and also on five-qubit device. In order to obtain the ground state energy of the negative hydrogen ion we used several local optimization methods to converge energy of the system to the energy minimum.

AKPIK 2: AKPIK Posters

Time: Monday 18:45–19:30 Location: P2/1OG

AKPIK 2.1 Mon 18:45 P2/1OG

Feature detection of grazing-incidence wide-angle X-ray scattering patterns by artificial neural networks — •Vladimir Starostin, Alessandro Greco, Alexander Hinderhofer, Alexander Gerlach, and Frank Schreiber — Institute of Applied Physics, University of Tübingen, Germany

Grazing-incidence wide-angle x-ray scattering (GIWAXS) is an indispensable tool for studying nanostructure surfaces and thin films. It is widely used in real-time studies of thin film growth. However, high acquisition rates of real-time experiments lead to enormous amounts of data to be analysed. For instance, a modern 2D X-ray detector has around 4.5 million of pixels and produces up to 6 Gb of data per second at the maximum frame rate of 750 Hz. In the future, these numbers will only increase and it may become unfeasible to analyze or even save unprocessed data. To address these problems, some automated tools need to be developed [1].

In this work, we present a machine learning approach that provides feature detection of GIWAXS images in an automated fashion. This simplifies the experimental data analysis and might enable on-the-fly preprocessing of GIWAXS data.

[1] Greco et al. *J. Appl. Cryst.* (2019). **52**, 1342–1347

AKPIK 2.2 Mon 18:45 P2/1OG

Real-Time Localization and Classification for Digital Microscopy using Single-Shot Convolutional Neural Networks — Martin Fränzl and •Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Germany

Common single particle tracking approaches work fast and reliable for images, where all objects have a sufficiently high signal to noise. Whenever the contrast in the images varies considerably over the particles and the signal-to-noise is low most simple techniques fail. We present a single shot neural network system based on the YOLO architecture for the classification and tracking of particles in optical microscopy data. The network is implemented in Python/Keras using the TensorFlow backend. The trained model is then exported to a GPU supported TensorFlow C library for real-time inference readily integrable in other programming languages such as MATLAB and LabVIEW. The network is able to reliably classify and localize several hundred objects in images of 416 × 416 pixels even at low signal to noise (SNR ∼ 1). As compared to previous work, our system is fast to allow for a real-time detection at 50 frames per second independent of the number of particles contained.

AKPIK 2.3 Mon 18:45 P2/1OG

Tensor network completion for gate set tomography — •Raphael Brieger[1], Ingo Roth[2], and Martin Kliesch[1] — [1]Institute for Theoretical Physics, Heinrich Heine University Düsseldorf, Germany — [2]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Germany

Flexible characterization techniques that quantify and identify noise under realistic assumptions are crucial for the development of near term quantum simulators.Gate set tomography (GST) has been proposed as a technique that simultaneously extracts tomographic information on an entire set of quantum gates, the state preparation and the measurements under minimal assumptions. We argue that the problem of reconstructing the gate set can naturally be cast as the problem of completing a translation-invariant matrix product state (MPS) from the knowledge of some of its entries. Such structured completion problems can be studied using the mathematical framework of compressed sensing. Extending recent results from the compressed sensing literature, we develop a new approach to the GST data processing task. We provide an MPS completion algorithm that can be used for the reconstruction of gate sets. Potential advantages of this approach are the ability to include physicality and low-rank constraints as well as prior knowledge on the gate implementations. We further discuss GST as a homogeneous polynomial optimization problem, where recovery guarantees are available at the cost of higher computational complexity. Our approach is a promising first step towards more scalable GST schemes amenable to theoretical guarantees.

AKPIK 2.4 Mon 18:45 P2/1OG

Evolution of Property and Bonding Maps — •Carl-Friedrich Schön and Matthias Wuttig — RWTH Aachen University, I. Physikalisches Institut (IA), Otto-Blumenthal-Straße, 52074 Aachen

Since picking up the first tools 2.5 million years ago, it has always been the goal of mankind to create materials that suit their needs best. While for the longest time any development in this field was driven by a "Cook'n'Look" approach, where new materials are discovered in a trial and error fashion, the means of modern physics and chemistry gave rise to the concept of material and property maps, which enabled a more focused approach.

An overview of material and property maps is presented, showcasing their individual advantages and drawbacks. The maps are evaluated as predictors for the electrical conductivity, the Grüneisen parameter, the effective coordination number, the Born effective charge and the optical dielectric constant, as well as to identify topological insulators and good thermoelectric materials. Furthermore, a link to the underlying bonding mechanisms of the materials shown in the maps is drawn, while a classification algorithm is utilized to assess the descriptive power of the maps and of chemical bonding itself.