

AKPIK 2: AKPIK Posters

Time: Monday 18:45–19:30

Location: P2/10G

AKPIK 2.1 Mon 18:45 P2/10G

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 P2/10G

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 P2/10G

Tensor network completion for gate set tomography —

●RAPHAEL BRIEGER¹, INGO ROTH², and MARTIN KLIESCH¹ — ¹Institute for Theoretical Physics, Heinrich Heine University Düsseldorf, Germany — ²Dahlem 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 P2/10G

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.