

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 MAUDET¹, VEERESH DESHPANDE¹, HANNO KRÖNCKE¹, and CATHERINE DUBOURDIEU^{1,2} —¹Institute Functional Oxides for Energy-Efficient Information Technology (EM-IFOX), Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — ²Freie Universität 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 GRECO¹, VLADIMIR STAROSTIN¹,CHRISTOS KARAPANAGIOTIS², ALEXANDER HINDERHOFER¹, ALEXANDER GERLACH¹, LINUS PITHAN³, SASCHA LIEHR⁴, FRANK SCHREIBER¹, and STEFAN KOWARIK⁴ — ¹Institut für Angewandte Physik, University of Tübingen, Auf der Morgenstelle 10, Tübingen 72076, Germany — ²Institut für Physik, Humboldt Universität zu Berlin, Newtonstrasse 15, Berlin 12489, Germany — ³European Synchrotron Radiation Facility, 71 Avenue des Martyrs, Grenoble 38000, France — ⁴Bundesanstalt 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 SiO₂ 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 Artificial 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 KOTTMANN¹, PATRICK HÜMBELI¹, MACIEJLEWENTEIN^{1,2}, and ANTONIO ACIN^{1,2} — ¹ICFO, Avinguda Carl Friedrich Gauss, 3, 08860 Castelldefels — ²ICREA, 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 processes 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.

$$f(J)=2x(0.1eV)/(h)=2x(15.6 \times 15.6)\text{Hz} \times 10^{11} \text{ neurons/brain.}$$

$f(J)=2x((1/64 \text{ Codons}) \times 15.6)\text{Hz} \times 10^{14} \text{ synapses/Neuron}$. The Josephson frequency $f(J)=15.6 \text{ Hz}$ is associated with the brain waves! For further AI-associated Interfaces can be found: On cosmology: $f(AI)=(69\% \text{ dark E.})/(4.5\% \text{ bar. Mat.})=15.3$. On the entropy: $f(AI)=1/(\text{entropy } 0.066)=e^{15.15}$. On the golden ratio Phi: $f(AI)=3\pi \times \text{Phi}(1.618)=15.3$. Conclusion: AI is a fractal 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 en-

ergy of negative hydrogen ion — •IVANA MIHÁLIKOVÁ^{1,2}, MARTIN FRIÁK^{1,2}, MATEJ PIVOLUSKA³, MARTIN PLESCH³, and MOJMIŘ ŠOB^{4,1,5} — ¹Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — ²Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Brno, Czech Republic — ³Institute of Computer Science, Masaryk University, Brno, Czech Republic — ⁴Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — ⁵Department 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.