AKPIK 3: Research with AI: Hardware, Software, Tools

Time: Tuesday 11:00–12:30 Location: H5

Invited Talk AKPIK 3.1 Tue 11:00 H5

3D Integration Towards Autonomous Optical Neural Networks — •Adrià Grabulosa, Anas Skalli, and Daniel Brunner — Institute Femto-ST, Université Marie et Louis Pasteur, CNRS UMR6174, 15B Avenue des Montboucons, Besançon, France.

In the last decades, modern electronic integrated circuits has reached a fundamental limit at 2 nm feature sizes. At the same time, emerging computing concepts such as neural networks (NNs), which are already playing a major role in modern societies, further amplifying this challenge. Adopting the third dimension is a promising strategy for achieving scalability of connections over the microchip's dimensions. Here, based on additive one- (OPP) and two-photon polymerization (TPP) processes and combined with direct-laser writing (DLW) settings, a complete toolbox comprising photonic waveguides, splitters and bends towards three-dimensional (3D) photonic integration is presented. The concept CMOS is validated by printing 3D photonic waveguides onto semiconductor (GaAs) substrates and silicon-on-insulator (SOI) platforms. Finally, we show first steps towards the 3D integration of a fully autonomous NN using spatially multiplexed modes of an injection locked large area vertical cavity surface emitting laser (LA-VCSEL) capable of performing NN tasks with >98% accuracy, fully realized in hardware using off-the-shelf, low energy consumption components. Overall, these building blocks are highly appealing for realizing fully-parallel and efficient communication throughout a densely-connected network, which are pivotal concepts for future NN computing topologies.

AKPIK 3.2 Tue 11:30 H5

Brain-inspired Computing with Gold Nanoparticle Networks: A Kinetic Monte Carlo Model — •Jonas Mensing and Andreas Heuer — Institute of physical Chemistry, University of Münster, Germany

Nanoparticles interconnected by insulating organic molecules exhibit nonlinear switching behavior at low temperatures. By assembling these nonlinear switches into a network and manipulating the inner charge transport dynamics via surrounding electrodes, the network can be functionalized to approximate functions such as Boolean Logic or model dynamical systems given the temporal dependence of input data. This makes nanoparticle networks promising candidates for neuromorphic computing and eventually bring machine learning applications on hardware.

We developed a kinetic Monte Calo simulation tool that applies established principles of single-electronics to model charge transport dynamics in nanoparticle networks. We demonstrate the network*s capability to approximate functions such as Boolean logic, perform nonlinear transformation of time dependent input signals, and forecast time series. These applications are evaluated using fitness metrics, enabling the optimization of surrounding electrode voltages to train the internal charge transport for a given task. The fitness measures are further analyzed in relation to system sizes, network disorder, or temporal scales. Furthermore, newly derived metrics enable us to link these design parameters to general nonlinear properties of the network.

AKPIK 3.3 Tue 11:45 H5

Discovery of the data structure as a way for prediction accuracy improvement — •Aliaksei Mazheika — independent researcher, Berlin, DE

High prediction accuracy of machine learning (ML) models is the main figure of merit of models efficiency. Usually this is achieved by choosing an optimal ML method, discovering the hyperparameters space, augmenting the data, etc. However, if a data set contains the data subsets significantly varying in their properties, addressing such heterogeneity can be pretty challenging task. Herewith a new method is presented in which improvement of prediction accuracy is achieved by discovering the heterogeneity of the data sets. This is done using a data mining method the subgroups discovery, in which the subsets of data are generated and discovered in terms of prediction accuracy improvement of local models in comparison to the global model within certain ML formalism. The application of this method showed its efficiency for classical data sets allowing for instance to solve the XOR problem staying on the level of logistic regression. Applying developed method for building ML models for a range of perovskite materials properties (lattice vector, tolerance factor) showed improvement of prediction accuracy for up to 50% for regression tasks, and up to 10% for classification. Also the new method was found to provide improved domains of applicability for ML models compared to previously proposed ones.

AKPIK 3.4 Tue 12:00 H5

Calculating the electronic structure of GaAs using Variational Quantum Algorithms — •Ivana Miháliková[1,2], Michal Krejčí[1,2], and Martin Friák[1] — [1]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Brno, Czech Republic

Simulating and characterizing physical systems is one of the most promising applications of quantum computing. In our research, we focused on electronic structure calculations of GaAs using quantum computer simulator. This work explores the binary crystal gallium arsenide, employing Variational Quantum Deflation (VQD) and the Subspace-Search Variational Quantum Eigensolver (SSVQE) to access the full energy spectrum. A tight-binding Hamiltonian is used to investigate the effects of optimization methods, hyperparameter tuning, and quantum circuit architecture on the performance of these variational quantum algorithms. Our findings show that higher-energy states require more iterations for accurate evaluation, with the Constrained Optimization BY Linear Approximation (COBYLA) method proving to be the most effective. Notably, SSVQE demonstrates robustness to hyperparameter settings, while VQD is highly sensitive requiring precise hyperparameter tuning for optimal performance.

AKPIK 3.5 Tue 12:15 H5

Photonics and A.I. Education Supported by Virtual Reality and Unreal Engine Contents — •Arash Rahimi-Iman — I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

3D interactive elements visualized in computer game engines combined with virtual or mixed reality (VR/XR) offer many possibilities to reach younger people. Here, we present one example of a virtual reality environment for gamification in the field of photonics and AI, created in the Unreal Engine UE5 for own teaching and training activities.

Thanks to modern information technologies, a plethora of ways exist which allow promoting topics of interest to a wider audience - among them digital games on platforms such as PCs and phones. While modern simulation software and sophisticated 3D visualization tools from all around typically address advanced users with a much more accurate science representation, simplified exploration spaces and toy experiments can create excitement at different age levels and attract potentially new students towards natural science topics based on fun and fascination.