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 H5; Poster P2)

Invited Talks

AKPIK 3.1	Tue	11:00–11:30	H5	**3D Integration Towards Autonomous Optical Neural Networks** — •Adrià Grabulosa, Anas Skalli, Daniel Brunner
AKPIK 4.1	Tue	14:00–14:30	H5	**The Scaling of Intelligence: From Transformers to Agentic AI** — •Oliver Mey
AKPIK 4.2	Tue	14:30–15:00	H5	**Inverse Design in Electromagnetics with Artificial Intelligence** — •Willie Padilla
AKPIK 4.3	Tue	15:00–15:30	H5	**Inverse design of lateral hybrid metasurfaces with machine learning** — •Rui Fang, Amir Ghasemi, Dagou Zeze, Koen Valk, Yuqing Jiao, Peter Zijlstra, Mehdi Keshavarz Hedayati

Invited Talks of the joint Symposium AI-driven Materials Design: Recent Developments, Challenges and Perspectives (SYMD)

See SYMD for the full program of the symposium.

SYMD 1.1	Mon	15:00–15:30	H1	**Learning physically constrained microscopic interaction models of functional materials** — •Boris Kozinsky
SYMD 1.2	Mon	15:30–16:00	H1	**GRACE universal interatomic potential for materials discovery and design** — •Ralf Drautz
SYMD 1.3	Mon	16:00–16:30	H1	**Multiscale Modelling & Machine Learning Algorithms for Catalyst Materials: Insights from the Oxygen Evolution Reaction** — •Nong Artrith
SYMD 1.4	Mon	16:45–17:15	H1	**Inverse Design of Materials** — •Hongbin Zhang
SYMD 1.5	Mon	17:15–17:45	H1	**Data-Driven Materials Science** — •Miguel Marques

Invited Talks of the joint Symposium AI in (Bio-)Physics (SYAI)

See SYAI for the full program of the symposium.

SYAI 1.1	Thu	9:30–10:00	H1	**Predicting interaction partners and generating new protein sequences using protein language models** — •Anne-Florence Bitbol
SYAI 1.2	Thu	10:00–10:30	H1	**Realizing Schrödinger's dream with AI-enabled molecular dynamics** — •Alexandre Tkatchenko
SYAI 1.3	Thu	10:30–11:00	H1	**Emergent behavior of artificial intelligence** — •Steffen Rulands
SYAI 1.4	Thu	11:15–11:45	H1	**AI in medical research - navigating complexity with AI** — •Daniel Truhn
SYAI 1.5	Thu	11:45–12:15	H1	**Computational Modelling of Morphogenesis** — •Dagmar Iber

Sessions

AKPIK 1.1–1.3	Sun	16:00–18:15	H2	**Hands-on Tutorial: AI Fundamentals for Research (joint session BP/TUT/DY/AKPIK)**

AKPIK 2.1–2.4	Tue	9:30–10:30	H5	**Machine Learning Prediction and Optimization Tasks**
AKPIK 3.1–3.5	Tue	11:00–12:30	H5	**Research with AI: Hardware, Software, Tools**
AKPIK 4.1–4.3	Tue	14:00–15:30	H5	**Focus: Applications of Deep Neural Networks**
AKPIK 5.1–5.19	Thu	15:00–16:30	P2	**Poster**
AKPIK 6.1–6.6	Thu	16:30–18:00	H5	**AI Methods for Materials Science**

AKPIK 1: Hands-on Tutorial: AI Fundamentals for Research (joint session BP/TUT/DY/AKPIK)

Artificial intelligence (AI) has become an essential tool in modern physics, enabling new approaches to data analysis, modeling, and prediction. This hands-on tutorial provides an accessible introduction to key AI concepts, emphasizing their practical applications in physics research.

Please bring your laptop. There will be limited power outlets in the room, so come with a fully charged battery.

Materials will be made available from 10.03.2025, accessible via the following options:

GitHub repository:
https://github.com/RedMechanism/DPG-SKM-2025-Tutorial-AI-Fundamentals-for-Research

ZIP file download:
https://jlubox.uni-giessen.de/getlink/fiAGRzcGTiCL3GZxk8WAjom4/

Participants are encouraged to download them ahead of time.

Organized by Jan Bürger (Aachen), Janine Graser (Duisburg), Robin Msiska (Duisburg/Ghent), and Arash Rahimi-Iman (Gießen), with support from Stefan Klumpp (Göttingen) and Tim Ruhe (Dortmund).

Time: Sunday 16:00–18:15 Location: H2

Tutorial AKPIK 1.1 Sun 16:00 H2

Introduction — Jan Bürger[1], •Janine Graser[2], Robin Msiska[2,3], and Arash Rahimi-Iman[4] — [1]ErUM-Data-Hub, RWTH Aachen University, Aachen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Department of Solid State Sciences, Ghent University, Ghent, Belgium — [4]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University Gießen, Gießen, Germany

The session begins with an overview of essential AI concepts, including neural networks, training methodologies, and key distinctions between AI models. Participants will gain a foundational understanding of AI principles and how these tools can be leveraged for various research challenges.

5 min. break

Tutorial AKPIK 1.2 Sun 16:40 H2

Hands-On Session 1 – Function Approximation — •Jan Bürger[1], Janine Graser[2], Robin Msiska[2,3], and Arash Rahimi-Iman[4] — [1]ErUM-Data-Hub, RWTH Aachen University, Aachen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Department of Solid State Sciences, Ghent University, Ghent, Belgium — [4]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University Gießen, Gießen, Germany

In the first half of the interactive session, participants will work with Jupyter Notebooks to explore practical applications of machine learning. They will train simple neural networks to predict a mathematical function, gaining hands-on experience in tuning key parameters. Since neural networks can typically be considered universal function approximators, this concept is effectively illustrated using a one-dimensional function, making it easy to visualize and understand.

5 min. break

Tutorial AKPIK 1.3 Sun 17:30 H2

Hands-On Session 2 – Classification and More — Jan Bürger[1], Janine Graser[2], •Robin Msiska[2,3], and Arash Rahimi-Iman[4] — [1]ErUM-Data-Hub, RWTH Aachen University, Aachen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Department of Solid State Sciences, Ghent University, Ghent, Belgium — [4]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University Gießen, Gießen, Germany

The session demonstrates how pre-trained models can simplify tasks such as classification, making them readily applicable to research. Typical examples include recognizing handwritten digits, which showcase the power of pretrained models in solving common challenges. As a preview of advanced topics, the tutorial concludes with brief examples of large language models (LLMs) and generative AI.

AKPIK 2: Machine Learning Prediction and Optimization Tasks

Time: Tuesday 9:30–10:30 Location: H5

AKPIK 2.1 Tue 9:30 H5

Attention space geometry — •Claudius Gros — Institute for Theoretical Physics, Goethe University Frankfurt

Attention involves comparing query and key vectors in terms of a scalar product, $\mathbf{Q} \cdot \mathbf{K}$, together with a subsequent softmax normalization. Classicaly, parallel/orthogonal/anti-parallel queries and keys lead to large/intermediate/small attention weights. Here we study expressive attention (EA), which is based on $(\mathbf{Q} \cdot \mathbf{K})^2$, the squared dot product. In this case attention is enhanced when query and key are either parallel or anti-parallel, and suppressed for orthogonal configurations. For a series of auto-regressive prediction tasks, we find that EA performs at least as well as the standard mechanism, dot-product attention (DPA). Increasing task complexity, EA is observed to outperform DPA with increasing margins, which also holds for multi-task settings. For a given model size, EA manages to achieve 100% performance for a range of complexity levels not accessible to DPA.

AKPIK 2.2 Tue 9:45 H5

Global Opimization of Atomic Structures in Extra Dimensions — •Casper Larsen[1], Sami Kaappa[2], Andreas Vishart[3], Thomas Bligaard[4], and Karsten Jacobsen[5] — [1]Technical University of München — [2]Tampere University — [3]Technical University of Denmark — [4]Technical University of Denmark — [5]Technical University of Denmark

This work formulates an approach to global optimization of atomic structures by use of an atomic descriptor extending the atoms with additional nonphysical degrees of freedom. These include chemical identity coordinates, atomic existence, and hyperspatial coordinates, all of which can be energetically minimized separately or simultaneously. The minimization is performed on a surrogate potential energy surface generated by Gaussian process regression trained on DFT calculations as part of a Bayesian optimization algorithm, where it is assured that all relaxational end states and training points are physically valid. The method is shown to successfully interpolate energy and force predictions from a training set of physically valid structures to structures with nonphysical coordinates. The inclusion of extra degrees of freedom significantly improves the efficiency of optimization of both clusters and bulk materials by circumventing energy barriers encountered in the conventional potential energy surface.

AKPIK 2.3 Tue 10:00 H5

Co-orchestration of multiple instruments for automated exploration of structure-property relationships in combinatorial libraries — •Boris Slautin[1], Utkarsh Pratiush[2], Ilia Ivanov[3], Yongtao Liu[3], Rohit Pant[4], Xiaohang Zhang[4], Ichiro Takeuchi[4], Maxim Ziatdinov[5], and Sergei Kalinin[2,5] — [1]University of Duisburg-Essen, Essen, Germany — [2]University of Tennessee, Knoxville USA — [3]Oak Ridge National Laboratory, Oak Ridge, USA — [4]University of Maryland, College Park, USA — [5]Pacific Northwest National Laboratory, Richland, USA

The advancement of combinatorial synthesis techniques has significantly accelerated the development of novel materials. However, closing the loop in materials design requires powerful approaches for characterizing the synthesized libraries. This is a non-trivial task, as characterization often involves revealing multiple methods.

We present a multimodal co-orchestration framework for autonomous combinatorial library characterization through the simultaneous coordination of various tools (e.g., Raman spectroscopy, SPM). The multimodal co-orchestration enables the real-time utilization of acquired knowledge about one property to accelerate the exploration of other properties measured by different methods. The capabilities of the proposed framework were validated by the co-orchestrating of the SPM and Raman techniques in the Sm-BiFeO3 combinatorial library. The workflow confirms its effectiveness in optimizing the exploration trajectory. The proposed framework is general and can be extended to multiple modalities and arbitrary dimensionality of signals.

AKPIK 2.4 Tue 10:15 H5

Data nexus vista: A research assistance framework for physics-informed descriptor engineering — •Kanchan Sarkar and Axel Gross — Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany

In today's fast-paced world, accurate modeling and prediction of complex systems are more crucial than ever, particularly for advancing modern technologies. In energy storage, for example, the design of materials with tailored properties for sustainable, next-generation devices is a critical goal. However, the vast materials space and intricate nature of materials data poses serious challenges for experimental and computational explorations, often likened to searching for a needle in a haystack. To address this, we present "Data Nexus Vista," a flexible framework for descriptor engineering. The framework offers four core functionalities: (1) adaptive preprocessing protocols for defining physically meaningful data transformations; (2) a feature selection interface that incorporates physics-based rules for improved interpretability; (3) diverse correlation analysis tools to uncover underlying physical mechanisms; and (4) workflows for developing interpretable models that balance physical validity with statistical robustness. By enabling thorough exploration of data-physical phenomena connections, this user-guided, modular approach ensures scientific rigor while addressing uncertainties in complex systems. Moreover, its adaptable design allows seamless application across diverse domains, from energy storage, surface science to nonlinear optical properties, advancing both scientific discovery and practical innovation.

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.

AKPIK 4: Focus: Applications of Deep Neural Networks

Time: Tuesday 14:00–15:30 Location: H5

Invited Talk AKPIK 4.1 Tue 14:00 H5

The Scaling of Intelligence: From Transformers to Agentic AI — •Oliver Mey — Vodafone Tech Innovation Center, Dresden, Germany

The 2024 Nobel Prize in Physics recognized fundamental contributions to artificial intelligence and highlighted its profound impact on all disciplines, including physics. Generative AI has become a central tool in science and beyond, and understanding its underlying principles, the forces driving its rapid progress, and its emerging applications opens the door to new scientific breakthroughs and transformative innovations. We trace the evolution from Moore's Law to the scaling principles that enable today's large-scale AI models. At the heart of this transformation lies the Transformer architecture, the foundation of large-scale language models (LLMs) that generate coherent, context-aware text. These models are evolving into multimodal systems that seamlessly integrate text, images and other data types, greatly expanding their capabilities. Retrieval-augmented generation (RAG) extends LLMs with dynamic memory, enabling access to external information. In parallel, new concepts for task-dependent scaling of computations allow LLMs to distribute computational effort based on task complexity, increasing their efficiency in reasoning and adaptive problem solving. These advances pave the way for AI systems that act as collaborative agents and are capable of context-aware, goal-oriented interactions. In this talk, I will provide an overview of these developments and discuss them in the context of their broader implications, setting the stage for further specialized discussions.

Invited Talk AKPIK 4.2 Tue 14:30 H5

Inverse Design in Electromagnetics with Artificial Intelligence — •Willie Padilla — Duke University, Durham, North Carolina, USA

Artificial electromagnetic materials (AEMs) have enabled exotic electromagnetic responses that are difficult or impossible to achieve with naturally occurring materials. However, as AEMs have become more complex, the relationship between their structure and resulting properties is increasingly less understood, or sometimes completely unknown. Deep neural networks (DNNs) have been shown to effectively infer the relationship between AEM geometry and their electromagnetic properties, using simulated training data. More recently, a type of DNN * termed a large language model (LLM) * has shown a remarkable ability to respond to complex prompts. This presentation explores the potential of DNNs and LLMs for the inverse design of AEMs. I present a LLM fine-tuned on simulated data that can predict electromagnetic spectra over a range of frequencies given a text prompt that only specifies the AEM geometry. In view of the great potential of deep learning for the future of AEM research, we review the status of the field, focusing on recent advances, open challenges, and future directions.

Invited Talk AKPIK 4.3 Tue 15:00 H5

Inverse design of lateral hybrid metasurfaces with machine learning — •Rui Fang[1], Amir Ghasemi[1], Dagou Zeze[1], Koen Valk[2], Yuqing Jiao[2], Peter Zijlstra[2], and Mehdi Keshavarz Hedayati[1] — [1]Durham University — [2]Eindhoven Technology University

The development of metasurface structural colour typically depends on laborious and time-consuming simulations such as Finite Element Method (FEM) or Finite-Difference Time-Domain (FDTD) simulation, along with human intuition for parameter adjustments, rendering it impractical for design optimization. In this context, we have introduced an innovative AI-assisted design process that circumvents the intricate simulations, allowing for a swift and precise correlation between metasurface parameters and colour coordinates. In this study, we have applied the model to the lateral hybrid design, a novel concept in metasurfaces proposed by our research group and demonstrated that the model can predict a structure tailored to achieve continuous colour coordinates with an accuracy of up to 97%. A noteworthy aspect of our discovery is that the model is capable of predicting the range of colours that can be generated from a single design of an active metasurface. Our deep learning approach proves to be a valuable tool in designing active metasurfaces for structural colours. This advancement contributes to the development of highly sensitive sensors, bringing tunable metamaterials closer to practical applications.

AKPIK 5: Poster

Time: Thursday 15:00–16:30 Location: P2

AKPIK 5.1 Thu 15:00 P2

Photonic Matrix-Vector Multiplication at the Quantum Limit of single photons — •Mingwei Yang[1,2], Okan Akyüz[2], Felix Kübler[2], Konrad Tschernig[1], Xavi Barcons[1,3], Enrico Stoll[2], and Janik Wolters[1,2] — [1]Deutsches Zentrum für Luft- und Raumfahrt, Institute of Optical Sensor Systems, Berlin, Germany. — [2]Technische Universität Berlin, Berlin, Germany. — [3]Humboldt-Universität zu Berlin, Berlin, Germany.

Photonic integrated circuits (PICs) have emerged as a promising solution for performing energy-efficient matrix multiplication and addition operations (MACs) in neural networks [1]. In this work, we demonstrate a 4x4 optical matrix-vector multiplication (MVM) using a mesh of Mach-Zehnder interferometers (MZIs), operating with attenuated laser pulses at the single-photon level. Using this as an example, we analyze the quantum limit of energy consumption of optical systems for classical machine learning. [1] Wetzstein, Gordon, et al. "Inference in artificial intelligence with deep optics and photonics." Nature 588.7836 (2020): 39-47.

AKPIK 5.2 Thu 15:00 P2

Machine Learning Optimization of Chiral Photonic Nanostructures — •Davide Filippozzi[1], Nicolas Roy[2], Alexandre Mayer[2], and Arash Rahimi-Iman[1] — [1]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany — [2]NaXys, Namur Institute for Complex Systems, University of Namur, Belgium

Deep learning (DL) and evolutionary algorithms (EA) as part of the machine learning (ML) domain have recently been well utilized for optimization purposes, such as for nanostructure design. Particularly, unintuitive problems can benefit from the potential abstraction levels that artificial Neural Networks (NNs) can achieve based on sufficient training and proper data. Reinforcement learning approaches promise to boost inference of solutions for complicated design requirements and specific functionalities.

We present a study that discusses the nano-pattern design optimization with a combination of DL and EA for a dielectric surface's preference for single-handed circularly polarized light in reflection or transmission. Advancing our previous simulations and algorithms [O. Mey and A. Rahimi-Iman, Phys. Status Solidi RRL 2022, 16, 2100571], the optimization in chiral dichroism and reflectivity for our metasurface's design is discussed. Such ML optimization can improve desirable features of unintuitive metamaterials and photonic nanostructures, as increasingly highlighted in up-to-date literature.

AKPIK 5.3 Thu 15:00 P2

Towards an ontology-based digital twin for graphene-based conductor materials — •Fabian Teichert[1,2,3], Leonhard Niemann[4,5], Florian Fuchs[1,2,3], Jörg Schuster[1,2,3], and Martin Köhne[4] — [1]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [2]Center for Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany — [3]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany — [4]Department of Advanced Technologies and Micro Systems, Robert Bosch GmbH, Renningen, Germany — [5]Faculty of Natural Sciences, Chemnitz University of Technology, Chemnitz, Germany

The „Platform Material Digital“ (www.materialdigital.de) advances digital twins within material science, based on a semantic description using ontologies. The aim is to digitally represent (new) materials, their properties and crucial processing steps. We are actively involved in this endeavour by digitalizing graphene-based conductor materials. An ontology is created and enriched with simulation data and experimental data, covering various aspects such as model parameters, preparation processes, and measurement processes. We create the following demonstrator use cases with a semantic data description: (1) the integration of our simulation methods as workflows within the „Platform Material Digital“, (2) an App to store, filter, and post-process our production and measurement processes and material properties of the graphene-based conductor materials.

AKPIK 5.4 Thu 15:00 P2

Machine learning to resolve the structure: Perovskites and related materials — •Ekaterina Kneschaurek, Vladimir Starostin, Valentin Munteanu, Constantin Völter, Damian Balaz, Mikhail Romodin, Maik Hylinski, Dmitry Lapkin, Ivan Zaluzhnyy, Alexander Hinderhofer, Alexander Gerlach, and Frank Schreiber — University of Tübingen, Tübingen, Germany

Recent advances in synthesis of novel materials used in solar cells, such as perovskites, are supported by structural analysis, using X-rays. To unravel the complexity of such materials, we utilize both *in situ* (studying crystallization kinetics) and *ex situ* (accessing phase composition) X-ray diffraction. The high-resolution scattering patterns are recorded by large 2D detectors, resulting in enormous amounts of data, which are difficult to analyze manually [1]. In some cases, there are no crystallographic information files (.cif) for the newly synthesized materials. An initial guess, based on the composition of the studied material, can estimate ranges of expected scattering signals from distinct phases. The deep learning (DL) model can detect Bragg peaks within the diffraction pattern, while the application of clustering and 2D Gaussian fitting enables the processing of complex data to be conducted more effectively. Preliminary data analysis of 2D patterns in real time can increase the efficiency of beamtimes and provide a feedback loop to optimize the parameters of the experiment.

[1] Hinderhofer, A., Greco, A., Starostin, V., Munteanu, V., Pithan, L., Gerlach, A., Schreiber, F. (2023). J. Appl. Cryst. **56**, 3-11.

AKPIK 5.5 Thu 15:00 P2

Balancing the Cart-Pole: Deep Q-Networks vs. Echo State Networks — •Igor Polonskiy, Atreya Majumdar, and Karin Everschor-Sitte — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

Balancing a pole on a moving cart by applying directional forces is a standard benchmark problem in reinforcement learning. Deep Q-Networks [1], which integrate reinforcement learning with neural networks, have been highly effective in solving this problem. However, their reliance on multiple hidden layers makes them computationally intensive and energy-demanding. Replacing these hidden layers with an Echo State Network reduces trainable parameters and energy consumption. In this study, we compare the performance of Deep Q-Networks and Echo State Networks on the Cart-Pole problem. We show that an Echo State Network-Q-Network combination, with sufficient size and runtime, can not only match but also surpass Deep Q-Networks in cumulative rewards and control success rates.

[1] V. Mnih et al., Nature 518, 529 (2015)

AKPIK 5.6 Thu 15:00 P2

Latent Measures of Memory and Stochasticity in Dynamical Systems: Murphy's Law of Tumbling Toast — •Janine Graser, Atreya Majumdar, Kübra Kalkan, Ross Knapman, and Karin Everschor-Sitte — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of DuisburgEssen, 47057 Duisburg, Germany

Murphy's Law, which suggests that "anything that can go wrong will go wrong," is often exemplified by toast landing butter-side down. In reality, a toast falling from a table can be described by Newtonian mechanics and is bound to fall on the butter side under standard conditions [1]. Here, the fall is modelled through its seemingly hidden aspects (table height and toast asymmetry because of the butter).

We revisit the tumbling toast problem using the data-driven machine learning tools - latent entropy and latent dimension -introduced by Horenko et al. [2]. We develop a Python-based implementation that characterizes the fall using these latent measures. This approach has broader applications in other dynamical systems, such as predicting and optimizing magnetic material properties.

[1] R. A. J. Matthews, Eur. J. Phys. 16 172 (1995)
[2] I. Horenko et al., Commun. Appl. Math. Comput. Sci. 16 267-297 (2021).

AKPIK 5.7 Thu 15:00 P2

Measurement of thermal conductivity and thermal diffusivity through spatial and temporal temperature gradients — •Junsheng Zhuo[2] and Stephanie Lippmann[1,2] — [1]Institute of Applied Physics, Friedrich Schiller University Jena, Jena, Thuringia, 07745, Germany — [2]Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Jena, Thuringia, 07743, Germany

To address the challenges of measuring thermal properties of metal, a new device is being developed to measure both thermal conductivity and thermal diffusivity quickly and accurately. The sample is heated directly using an electromagnetic induction furnace, avoiding thermal resistance issues. High-resolution infrared cameras capture temperature distribution with ultra-short time and space intervals, allowing for precise thermal conductivity and diffusivity measurements. Mineral oil is used for cooling, enabling rapid heat transfer. This device calculates temperature-dependent thermal conductivity using spatial temperature gradients and heat flow, based on Fourier's law assisted by fitting, statistics, and machine learning, while thermal diffusivity is derived from real-time transient temperature gradients using the inverse method. Specific heat capacity is then calculated from these two values.

AKPIK 5.8 Thu 15:00 P2

Deterministic Model of Multi-Agent Boltzmann Q-Learning: Transient Dynamics, Feedback Loops, and Non-Convergence — •David Goll[1], Jobst Heitzig[2], and Wolfram Barfuss[3] — [1]Humboldt University of Berlin — [2]Potsdam Institute of Climate Impact Research — [3]University of Bonn

Multi-Agent Reinforcement Learning involves interacting agents whose learning processes are indirectly coupled through their shared environment, giving rise to emergent, collective dynamics that are sensitive to initial conditions and parameter variations. A Complex Systems approach, which examines dynamic interactions in multi-component systems, can uncover the underlying dynamics by constructing deterministic, approximate models of stochastic algorithms. In this work, we show that even in the simplest case of independent Q-learning with a Boltzmann exploration policy, previous models fail to capture actual learning behaviour. Specifically, the dynamics of the Q-space—representing agents' state-action value estimates—cannot be directly reduced to the lower-dimensional policy space representing their strategies, as assumed in earlier models. By explicitly incorporating agents' update frequencies, we propose a new discrete-time model that captures the observed behaviours and uncovers a fundamentally more complex dynamical landscape. We demonstrate the utility of this approach by applying it to the Prisoner's Dilemma, where our model distinguishes transient states, which might be mistaken for equilibria, from true equilibria. Furthermore, we show that varying hyperparameters, such as the discount factor, can prevent convergence to a joint policy.

AKPIK 5.9 Thu 15:00 P2

Noisy quantum computing of electronic structure of crystals — •Vojtěch Vašina[1,2], Ivana Miháliková[1], and Martin Friák[1] — [1]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic — [2]Brno University of Technology, Brno, Czech Republic

Quantum computing is currently emerging as a useful paradigm for solving highly complex computational problems. Current quantum computers are unfortunately too noisy to provide sufficient accuracy, and quantum-classical hybrid algorithms emerged as a solution. Variational Quantum Eigensolver (VQE) has gained significant attention for addressing challenges in quantum chemistry, material science, etc. VQEs typically use multiple optimization methods, and the correct choice of optimization method can significantly impact performance. In our study, we focused on the comparison of multiple optimization methods used in VQE when applied to the electronic structure of crystals. The quantum part of VQE ran on a classical simulator with imported noise models from real quantum computers from the IBM Quantum Platform.

AKPIK 5.10 Thu 15:00 P2

Advancing Digital Transformation in Research on Uni-

verse and Matter in Germany — Martin Erdmann[1], •Jan M. Bürger[1], Banjamin Fischer[1], Stefan Fröse[2], Judith Steinfeld[1], and Angela Warkentin[1] — [1]RWTH Aachen University — [2]TU Dortmund University

Research on Universe and Matter (ErUM) at major infrastructures such as CERN or large observatories, jointly conducted with university groups, is an important driver for the digital transformation. In Germany, about 20,000 scientists are working on ErUM-related sciences and can benefit from actual methods of artificial intelligence. The central networking and transfer office ErUM-Data-Hub provides support by designing, organizing and performing schools and workshops for young and expert scientists in the areas of big data, machine learning, sustainable computing and many more. We present the actual achievements of the ErUM-Data-Hub in the German ErUM community.

AKPIK 5.11 Thu 15:00 P2

The graphene resonant metasurface substrate in near-zero refractive index regime to control the surface plasmon-polariton propagation length — •Zoya Eremenko — Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Deutschland

The study goal is to identify and investigate conditions for controlling the propagation length of graphene surface plasmon-polaritons (SPP) through the utilization of hybrid graphene-dielectric metasurfaces. We study the spectral characteristics of resonant multipole modes in all-dielectric metasurface using the photonic crystal approach, metasurface unit cell modelling approach and implement these approaches by the commercial software Comsol Multiphysics 6.2. For controlling the propagation length of graphene SPPs we used all-dielectric metasurface as a substrate of graphene layer in a near-zero refractive index regime. The determined the parameters of the near-zero refractive index regime for the studied metasurface, which is crucial for achieving the main project goal of controlling SPP propagation length in the graphene layer. Knowing the effective refractive index of the metasurface unit cell in the near-zero regime, these values are used in Comsol modeling the hybrid metasurface as a graphene layer substrate to calculate the SPP propagation length.

AKPIK 5.12 Thu 15:00 P2

Development of a Parametric Design Program for Building Construction Elements using Artificial Intelligence — •Artem Burdin — Moscow, Russia

Thesis: The aim of this research is to develop a parametric design program for building construction elements using artificial intelligence, focusing on the application of modern IT and artificial intelligence in physics-based modeling and simulation. The program will enable the creation of complex building structures, such as bridges, tunnels, and high-rise buildings, with increased accuracy and efficiency. Key objectives: * Analyze the current state of parametric design in building construction * Develop a parametric design program using artificial intelligence and machine learning algorithms * Implement the program using a suitable programming language and software * Test and validate the program using real-world examples * Evaluate the program's performance and potential applications in the construction industry Expected outcomes: * A parametric design program capable of generating complex building structures with increased accuracy and efficiency * A comprehensive analysis of the current state of parametric design in building construction * A detailed evaluation of the program's performance and potential applications in the construction industry * Contributions to the development of artificial intelligence and modern IT in physics-based modeling and simulation Keywords: parametric design, building construction, artificial intelligence, machine learning, physics-based modeling, simulation, computer-aided design (CAD), construction industry.

AKPIK 5.13 Thu 15:00 P2

Working group on physics, modern Information technologies and artificial Intelligence — •Adam Barakhoev — Moscow, Russia

Artificial intelligence and modern computer infrastructure are changing the approach to physics, combining powerful computational methods with experiments. These innovations help scientists process large amounts of data, automate complex tasks, and make accurate predictions. One of the important achievements is the use of artificial intelligence to improve physical experiments, especially in quantum mechanics and optical systems. Machine learning algorithms can predict results based on incomplete data and help set up experiments in real time, which significantly increases their efficiency and accuracy. Also, modern OT technologies, such as cloud services and high-performance computing, are important for managing the large-scale modeling needed in modern physics research.

AKPIK 5.14 Thu 15:00 P2

Autonomous Vehicles: Technologies and Challenges — •Nikita Timoshin — Moscow, Russia

Autonomous vehicles are transforming transportation with technologies such as artificial intelligence (AI), machine learning, and advanced sensor systems like LiDAR, radar, and cameras. These vehicles rely on AI to make real-time decisions, using data from various sensors through sensor fusion for accurate environmental perception. Communication networks like V2X (Vehicle-to-Everything) and 5G enable vehicles to interact with infrastructure and other vehicles.

The benefits include enhanced safety by reducing human error, improved traffic efficiency, and increased mobility for people with disabilities. However, challenges such as sensor limitations in adverse conditions, high computational demands, and ethical dilemmas about decision-making in critical situations remain. Additionally, regulatory and privacy concerns need to be addressed. As autonomous vehicles integrate with smart cities, they could significantly reshape urban mobility.

AKPIK 5.15 Thu 15:00 P2

Experimental examination of the validity of the Turing test for considering Artificial Intelligence as having subjectivity — •Lev Gelbart and Alexey Iakovlev — Moscow, Russia

The speed of development of Artificial Intelligence (AI) raises questions about its subjectivity and thinking. Alan Turing, who set the criteria for thinking, did not consider subjectivity. There are sharp discussions on this topic, for example, Doctor of Law Valery Zorkin, professor at MSU, opposes endowing AI with subjectivity, emphasising humanism.

It should also be taken into account that the Turing test may be invalid if we consider people, who are not capable of passing it. For example, a study by Alan Ropper (2010) showed that patients in a vegetative state can demonstrate brain activity, but are clearly unable to pass the Turing test, which does not detract from their human value.

We have considered, whether a machine can pass a test designed for humans. Machines are thought to not be able to adequately mimic emotions, so we tested three chatbots (Lily, AI Chat, ChatGPT) for emotional intelligence using the IDRlabs test. All chatbots performed above the average of humans (77.27%, 68.87%, 64.6%), but this, obviously, does not make them subjects of law.

Conclusion: the Turing test is not valid for assessing the subjectivity of AI.

AKPIK 5.16 Thu 15:00 P2

Unmanned transportation in the field of cargo transportation and its contribution to industry. — •Alexey Platonov — Moscow, Russia

In recent years, the transportation industry has witnessed a transformative shift towards automation and innovation, with unmanned transportation systems emerging as a pivotal force in cargo logistics.

Unmanned transportation significantly improves safety in cargo movement. By reducing the reliance on human drivers, the industry can mitigate the risks associated with human error, a leading cause of accidents in transportation.

The integration of LiDAR into cargo transportation also opens up new avenues for delivery services.

It is worth considering that the active introduction of unmanned vehicles in cargo transportation is beginning. Several test shipments of real orders were made on KamAZ-5490 trucks without direct driver control. There was only a mechanic controller in the cockpit, who checked the performance of the systems.

By enhancing efficiency, improving safety, and fostering innovation, these technologies are set to revolutionize the logistics landscape, proving that the future of transportation is indeed unmanned.

AKPIK 5.17 Thu 15:00 P2

Crawler-motor grader — •Vyacheslav Kharchevnikov — Moscow, Russia

An overview of the relevance and necessity of developing a crawler-mounted motor grader. A description of the problems that this equipment solves in the construction and road sector. An analysis of existing

models of motor graders, including wheeled and tracked versions, their advantages and disadvantages. Defining the main goal of the project - to create an effective crawler-mounted motor grader. Setting the tasks necessary to achieve the goal, such as improving the cross-country ability and stability of the equipment. A detailed description of the design of a crawler-mounted motor grader, including the features of the chassis, control system and attachments.

An analysis of the economic feasibility of introducing a crawler-mounted motor grader, a comparison with traditional models, an assessment of production and operating costs. An assessment of the environmental impact of using a crawler-mounted motor grader, measures to reduce emissions and reduce noise. Summarizing the research, assessing the results achieved and prospects for further development and implementation of a crawler-mounted motor grader.

AKPIK 5.18 Thu 15:00 P2

Development of a design solution for automating a set of tasks in the production preparation subsystem of an automated control system for a small construction company — •Tikhon Shabrov — Moscow, Russia

automation of processes for small companies use of new technologies

AKPIK 5.19 Thu 15:00 P2

Acceleration of crystal structure relaxation with Deep Reinforcement Learning — •Elena Trukhan, Efim Mazhnik, and Artem R. Oganov — Moscow, Russia

We introduce a Deep Reinforcement Learning (DRL) model for the structure relaxation of crystal materials and compare different types of neural network architectures and reinforcement learning algorithms for this purpose. Experiments are conducted on Al-Fe structures, with potential energy surfaces generated using EAM potentials. We examine the influence of hyperparameter settings on model performance and benchmark the best-performing models against classical optimization algorithms. Additionally, the model's capacity to generalize learned interaction patterns from smaller atomic systems to more complex systems is assessed. The results demonstrate the potential of DRL models to enhance the efficiency of structure relaxation compared to traditional methods.

AKPIK 6: AI Methods for Materials Science

Time: Thursday 16:30–18:00 Location: H5

AKPIK 6.1 Thu 16:30 H5

Bayesian Optimization for High-Resolution Transmission Electron Microscopy — •Xiankang Tang[1], Lei Jin[2], Yixuan Zhang[1], Rafal Dunin-Borkowski[2], and Hongbin Zhang[1] — [1]Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany — [2]Ernst Ruska-Centrum für Mikroskopie und Spectroskopie mit Elektronen, FZ Jülich, 52428 Jülich, Germany

Advances in machine learning technologies make it possible to automatize material characterizations, indispensable for the near-future implementation of autonomous experimentation for solid-state materials. High-resolution transmission electron microscopy (HRTEM) allows the study of the atomic structure of solid materials with sub-Angstrom resolution. By matching experimental and simulated images, unknown experimental parameters and crystal structures can be determined. However, this process entails strong domain expertise and can be time-consuming. In this work, we implement a Bayesian optimization-based approach to automatize the image analysis processes. Combined with some prior information, such as the experimentally measured aberration, the 3D crystal structure of the specimen can be reconstructed from a single HRTEM image. Specifically, by defining the mean square error(MSE) of pixel intensity values between experimental and simulated images, our method effectively captures both global and local image features. This approach not only achieves an exact match in absolute image contrast but also identifies unknown experimental parameters, optimizes atomic positions, and reveals surface morphology at atomic resolution.

AKPIK 6.2 Thu 16:45 H5

Synthetic Data Generation for Enhanced Segmentation of Electron Microscopy Images — •Amir Omidvarnia[1], Ali Ghaznavi[2], Junbeom Park[1], Shibabrata Basak[1], and Simone Köcher[1] — [1]Institute of Energy Technologies - Fundamental Electrochemistry (IET-1), Forschungszentrum Jülich GmbH, 52428 Jülich, Germany — [2]Federal Institute for Materials Research and Testing (BAM), 12205 Berlin, Germany

Monitoring structural changes in materials via operando electron microscopy (EM) is crucial for understanding the material's changes under operating conditions, which directly impacts its durability and performance. However, accurate segmentation of features such as cracks or pores in EM time-series data requires extensive labeled datasets, which are challenging to produce due to the labor-intensive, subjective nature of manual annotation. Our research addresses this limitation by exploring different synthetic data generation techniques that can effectively supplement scarce annotated data and improve segmentation outcomes. We evaluate multiple synthetic image generation approaches to enhance the training dataset for U-Net models aimed at segmenting EM time-series data: (1) deep convolutional generative adversarial networks (DCGAN) to produce realistic textures; (2) time-varying image synthesis that mimics the temporal development of features and introduces artificial features to simulate structural imperfections; and (3) standard data augmentation methods. These methods are evaluated in generating training data for EM image segmentation from a limited set of EM images.

AKPIK 6.3 Thu 17:00 H5

Neural Networks in Surface Crystallography: A New Paradigm for GIWAXS Analysis — •Erwin Pfeiler[1], Vladimir Starostin[3], Alexander Hinderhofer[3], Roland Resel[2], Frank Schreiber[3], and Stefan Kowarik[1] — [1]University of Graz, Austria — [2]TU Graz, Austria — [3]University of Tübingen, Germany

Thin film materials are essential to modern technology, with grazing incidence X-ray diffraction (GIWAXS) being the primary method for resolving their crystal structure. However, the current data analysis process is often slow and labor-intensive, frequently requiring more time and resources than the GIWAXS measurements themselves. Accelerating this bottleneck is critical for enabling automated materials discovery.

In this work, we present an AI-driven approach utilizing neural networks to streamline and enhance GIWAXS analysis. Our model predicts unit cell dimensions (a, b, c) and angles (α, β, γ) directly from the positions of Laue reflections. Additionally, it identifies the Miller indices of the contact plane, providing insights into the film texture.

Using both simulated GIWAXS data and real-world examples, we demonstrate the neural network's potential to significantly accelerate the analysis process, delivering accurate structural predictions with sub 0.01 Å precision.

AKPIK 6.4 Thu 17:15 H5

Reflectivity Analysis with AI: The LISA Data Pipeline at P08/DESY — •Julia Kobus[1,2], Lukas Petersdorf[1,2], Svenja Hövelmann[1,2], Alexander Hinderhofer[3], Vladimir Starostin[3], Chen Shen[4], Florian Bertram[4], Linus Pithan[4], Frank Schreiber[3], and Bridget Murphy[1,2,4] — [1]Institute of Experimental and Applied Physics, Kiel University, Leibnizstr. 19, 24118 Kiel, Germany — [2]Ruprecht-Haensel Laboratory, Olshausenstr. 40, 24098 Kiel, Germany — [3]University of Tübingen, 72076 Tübingen, Germany — [4]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany

We present a data analysis pipeline that is under development within TA3 of DAPHNE4NFDI for the LISA instrument at the P08 beamline at DESY. This pipeline is adapted from the development on solid surface XRR AI analysis to be used for liquid surfaces and interfaces. The pipeline aims at performing data reduction and subsequent analysis for reflectivity measurements using AI-based models. This approach increases measurement efficiency by processing data in real time, allowing flexible adjustments during the experiment and providing immediate insights. This will help users make better-informed decisions for subsequent measurements. The pipeline also will make advanced data analysis accessible to less experienced users. Our work will demonstrate the potential of AI to transform experimental workflows and

data interpretation, and provides a blueprint for similar developments in the scientific community.

AKPIK 6.5 Thu 17:30 H5

Prediction of Infrared Spectra of organic molecules with Active Learning — •Gusein Bedirkhanov[1], Nitik Bhatia[1], Ondrej Krejci[2], and Patrick Rinke[1,2] — [1]Department of Physics, Technical University of Munich, Germany — [2]Department of Applied Physics, Aalto University, Finland

Infrared (IR) spectroscopy is a valuable tool for understanding catalytic processes, but interpreting experimental spectra is challenging due to the strong influence of the species environment. Ab initio molecular dynamics (AIMD) offers accurate theoretical spectra, accounting for anharmonic effects, but at a high computational cost. Machine-learned interatomic potentials (MLIPs), such as MACE [1], provide an alternative to AIMD, enabling accurate and fast IR spectra predictions. To reduce the amount of training data, we have established the active learning method PALIRS [2] (a Python-based active learning code for infrared spectroscopy). PALIRS predicts IR spectra of organic molecules essential in catalytic processes accurately, with peak positions matching experiment within 20cm^{-1}. We aim to further improve the efficiency of PALIRS, using only a hundredth of DFT data in comparison with AIMD, through optimization of MACE training strategies. We will inspect various combinations of transfer learning and conventional iterative training to find the ideal match between training time and final MLIP accuracy.

[1] I. Batatia *et al.*, Adv. Neural inf. Process. Syst. (2022).

[2] N. Bhatia *et al.*, GitHub (2024), `gitlab.com/cest-group/PALIRS`

AKPIK 6.6 Thu 17:45 H5

Towards AI-assisted high-throughput thin film research workflow — •Dmitry Lapkin, Roody Nasro, Constantin Völter, Valentin Munteanu, Alexander Hinderhofer, Alexander Gerlach, and Frank Schreiber — University of Tübingen

The compositional optimization of new materials necessitates the high-throughput screening of a multitude of compositions, which must be investigated to elucidate the non-linear and non-monotonic structure-property-composition dependencies. In this regard, data-driven material science enables researchers to accelerate the identification of new materials with desired properties for specific applications by efficiently exploring vast material spaces. Such high-throughput data-driven studies comprise two key elements: the combinatorial preparation of suitable sample libraries spanning wide compositional ranges, and the high-throughput screening of the structure and properties of the synthesized samples.

In this work, we present a complete workflow for high-throughput studies of thin films. A specially designed vacuum deposition chamber enables the production of gradient thin films suitable for high-throughput screening. Surface-sensitive X-ray scattering methods available at modern X-ray sources comprise a convenient tool for resolving the thin film structure with ultimate resolution and high speed, while the developed AI-based approaches provide on-the-fly analysis of the collected X-ray scattering data.