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 BEY/0127; Poster P5)

Invited Talks

AKPIK 3.4	Tue	11:45–12:15	BEY/0127	**Model-free training of optical neural networks based on multimode semiconductor lasers** — •Anas Skalli, Satoshi Sunada, Mirko Goldmann, Marcin Gebski, Nasibeh Haghighi, Stephan Reitzenstein, James A. Lott, Tomasz Czyszanowski, Daniel Brunner
AKPIK 3.5	Tue	12:15–12:45	BEY/0127	**Virtual Reality Gamification for Photonics, AI and More** — •Arash Rahimi-Iman
AKPIK 4.1	Tue	14:00–14:30	BEY/0127	**Beyond the Hype: Can AI Truly Transform Photonics?** — •Mehdi K. Hedayati
AKPIK 4.2	Tue	14:30–15:00	BEY/0127	**Machine–learning assisted design of metasurfaces** — Lukas Mueller, Alexander Wolff, Janis Krieger, Steffen Klingel, Ralf Stemler, •Marco Rahm

Invited Talks of the joint Symposium The Sustainability Challenge: A Decade of Transformation (SYSC)

See SYSC for the full program of the symposium.

SYSC 1.1	Mon	15:00–15:30	HSZ/AUDI	**Open-Endedness and Community-Based Approaches to Sustainability Challenges** — •Hiroki Sayama
SYSC 1.2	Mon	15:30–16:00	HSZ/AUDI	**Education as a Social Tipping Element: Evidence from Climate and Physics Education Research** — •Thomas Schubatzky
SYSC 1.3	Mon	16:00–16:30	HSZ/AUDI	**Mechanistic and Material Perspectives on Enzymatic Hydrolysis of Semicrystalline Polyesters** — •Birte Höcker
SYSC 1.4	Mon	16:45–17:15	HSZ/AUDI	**Decarbonization Options for Industry** — •Uwe Riedel
SYSC 1.5	Mon	17:15–17:45	HSZ/AUDI	**Impacts of Cosmic Dust and Space Debris in the Terrestrial Atmosphere** — •John Plane

Invited Talks of the joint Symposium AI and Data Challenges behind Emerging Self-Driving Laboratories (SYAI)

See SYAI for the full program of the symposium.

SYAI 1.1	Thu	9:30–10:00	HSZ/AUDI	**Data and Experimental Foundations for Reliable Self-Driving Laboratories** — •Dr. Marcus Tze-Kiat Ng
SYAI 1.2	Thu	10:00–10:30	HSZ/AUDI	**Digital Catalysis - AI for Experiment Planning and Control** — •Christoph Scheurer
SYAI 1.3	Thu	10:30–11:00	HSZ/AUDI	**Autonomous, Data-Driven Workflows for Materials Acceleration Platforms with pyiron** — •Jan Janssen, Joerg Neugebauer

SYAI 1.4	Thu	11:15–11:45	HSZ/AUDI	**Machine Learning for Autonomous Optimization and Discovery of Materials** — •Pascal Friederich
SYAI 1.5	Thu	11:45–12:15	HSZ/AUDI	**Transforming Our View on Transformers in the Sciences** — •Kevin Maik Jablonka

Sessions

AKPIK 1.1–1.4	Sun	16:00–18:15	HSZ/0003	**Tutorial: Machine Learning Use Cases in Materials Science (joint session AKPIK/TUT)**
AKPIK 2.1–2.5	Tue	9:30–10:45	BEY/0127	**Machine Learning Prediction and Optimization Tasks**
AKPIK 3.1–3.5	Tue	11:00–12:45	BEY/0127	**Research with AI: Hardware, Software, Tools**
AKPIK 4.1–4.4	Tue	14:00–15:30	BEY/0127	**Focus: Deep Learning in Electromagnetics Research**
AKPIK 5.1–5.15	Thu	15:00–16:30	P5	**Poster**
AKPIK 6.1–6.7	Thu	16:45–18:30	BEY/0127	**AI Methods for Physics and Materials Science**

AKPIK 1: Tutorial: Machine Learning Use Cases in Materials Science (joint session AKPIK/TUT)

Artificial intelligence (AI) tools are increasingly shaping research in materials science and physics by enabling advanced data analysis, modeling, and predictive capabilities.

This tutorial presents three practical use cases that demonstrate how machine learning methods can support materials science research.

Time: Sunday 16:00–18:15 Location: HSZ/0003

Tutorial AKPIK 1.1 Sun 16:00 HSZ/0003
Welcome Remarks Arbeitskreis Physik, moderne Informationstechnologie und Künstliche Intelligenz — DPG AKPIK and •Arash Rahimi-Iman — Deutsche Physikalische Gesellschaft e.V.

Inspired by last year's meeting program in Regensburg, March 2025, our interdisciplinary Working Group on Physics, Modern IT and Artificial Intelligence, the AKPIK, again offers a research-focused "AKPIK Day" on Tuesday during the upcoming conference. Together with the practical use cases of machine learning presented in this tutorial session, as well as the presentations and poster session planned for Thursday, we hope to encourage many conference attendees to engange scientifically in the areas of the AKPIK.

Tutorial AKPIK 1.2 Sun 16:05 HSZ/0003
A practical machine learning case study in materials science: Stumbling blocks, lucky breaks, and helpful colleagues — •Max Grossmann, •Malte Grunert, and Erich Runge — Institute of Physics and Institute of Micro- and Nanotechnologies, Technische Universität Ilmenau, 98693 Ilmenau, German

Machine learning projects in materials science are often exciting at first, but quickly encounter practical challenges. In this tutorial, we present a hands-on case study from our group and walk through the entire process, from the initial idea to building a dataset to training a working model. Rather than focusing solely on technical details, we highlight the stumbling blocks, unexpected insights, helpful colleagues, and lucky coincidences that shaped the project. We discuss the most important aspects of starting a machine learning project in physics or materials science, such as choosing a meaningful target property, designing a reliable dataset, avoiding common pitfalls, and identifying situations where simple approaches are as effective as advanced ones. Our goal is to provide an honest, accessible, and experience-driven introduction and guidance to researchers considering venturing into machine learning for the first time – the kind of guidance we wish we had when we started.

5 min. break

Tutorial AKPIK 1.3 Sun 16:50 HSZ/0003
Machine Learning-based Analysis of Electron Microscopy Images: Preprocessing and Synthetic Data Generation — •Amir Omidvarnia — Forschungszentrum Jülich, Jülich, Germany

In this tutorial session, participants will learn how to prepare electron microscopy (EM) images for machine learning (ML) analysis using a series of Jupyter Notebook demonstrations. The tutorial illustrates essential preprocessing steps such as denoising, normalization, and contrast enhancement using Python. The session then transitions to synthetic EM data generation, showing how classical augmentation and modern generative models can create controlled datasets that mimic real data. By observing these live examples, attendees will gain a conceptual understanding of how preprocessing pipelines and synthetic data strategies can be used for ML-based EM analysis.

5 min. break

Tutorial AKPIK 1.4 Sun 17:35 HSZ/0003
Machine Learning-based Analysis of Electron Microscopy Images: Segmentation — •Amir Omidvarnia — Forschungszentrum Jülich, Jülich, Germany

The second session focuses on segmentation of EM images using modern deep-learning architectures. Through a step-by-step Jupyter Notebook demonstration, the tutorial walks through the training and evaluation of a U-Net style segmentation model. Participants will see real examples of common challenges in EM segmentation, such as low contrast, overlapping nanoscale structures, and label ambiguity. By the end of the session, attendees will have an implementation-oriented understanding of how segmentation pipelines are built and validated in practice.

AKPIK 2: Machine Learning Prediction and Optimization Tasks

Time: Tuesday 9:30–10:45 Location: BEY/0127

AKPIK 2.1 Tue 9:30 BEY/0127
Bayesian Optimization for Mixed-Variable Problems in the Natural Sciences — •Yuhao Zhang[1], Ti John[2], Matthias Stosiek[1], and Patrick Rinke[1,3] — [1]School of Natural Sciences Physics Department, Technical University of Munich, Germany — [2]Department of Computer Science Aalto University, FInland — [3]Munich Center for Machine Learning, Germany

Optimizing expensive black-box objectives over mixed search spaces is a common challenge across the natural sciences. Bayesian optimization (BO) offers sample-efficient strategies through probabilistic surrogate models and acquisition functions. However, its effectiveness diminishes in mixed or high-cardinality discrete spaces, where gradients are unavailable and optimizing the acquisition function becomes computationally demanding. In this work, we generalize the probabilistic reparameterization (PR) approach of Daulton et al. to handle non-equidistant discrete variables, enabling gradient-based optimization in fully mixed-variable settings with Gaussian process surrogates. With real-world scientific optimization tasks in mind, we conduct systematic benchmarks on synthetic and experimental objectives to obtain an optimized kernel formulations and demonstrate the robustness of our generalized PR implementation. We additionally show that, when combined with a modified BO workflow, our approach can efficiently optimize highly discontinuous and discretized objective landscapes. This work establishes a practical BO framework for addressing fully mixed optimization problems encountered in the natural sciences.

AKPIK 2.2 Tue 9:45 BEY/0127
Overparametrization bends the landscape: BBP transitions at initialization in simple Neural Networks — •Brandon Livio Annesi, Chiara Cammarota, and Dario Bocchi — Sapienza Univeristy, Rome Italy

High-dimensional non-convex loss landscapes play a central role in the theory of Machine Learning. Gaining insight into how these landscapes interact with gradient-based optimization methods, even in relatively simple models, can shed light on this enigmatic feature of neural networks. In this talk, I will focus on a prototypical simple learning problem, which generalizes the Phase Retrieval inference problem by allowing the exploration of overparametrized settings. Using techniques from field theory, we analyze the spectrum of the Hessian at initialization and identify a Baik*Ben Arous*Péché (BBP) transition in the amount of data that separates regimes where the initialization is informative or uninformative about a planted signal. Crucially, we demonstrate how overparameterization can bend the loss landscape, shifting the transition point, even reaching the information-theoretic weak-recovery threshold in the large overparameterization limit, while also altering its qualitative nature. We distinguish between continuous and discontinuous BBP transitions and support our analytical predictions with simulations. In the case of discontinuous BBP transi-

tions strong finite-N corrections allow the retrieval of information at a signal-to-noise ratio (SNR) smaller than the predicted BBP transition. In these cases we provide estimates for a new lower SNR threshold that marks the point at which initialization becomes entirely uninformative.

AKPIK 2.3 Tue 10:00 BEY/0127

Training convolutional neural networks with the forward - forward algorithm — •Matthias Schröter[1,2], Frauke Alves[3], and Riccardo Scodellaro[3] — [1]Institute for Diagnostic and Interventional Radiology, University Medical Center Göttingen, Robert Koch-Straße 40, 37075 Göttingen, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, 37075 Göttingen, Germany — [3]Translational Molecular Imaging, Max Planck Institute for Multidisciplinary Sciences, 37075 Göttingen, Germany.

Recent successes in image analysis with deep neural networks are achieved almost exclusively with Convolutional Neural Networks (CNNs) trained using the backpropagation (BP) algorithm. In a 2022 preprint, Geoffrey Hinton proposed the Forward - Forward (FF) algorithm as a biologically inspired alternative, where positive and negative examples are jointly presented to the network and training is guided by a locally defined goodness function. Here, we extend the FF paradigm to CNNs. This talk compares FF and BP training across different datasets (MNIST, CIFAR 10, CIFAR 100) discusses different optimization strategies, and provides insights into the inner workings of FF trained networks using Class Activation Maps.

AKPIK 2.4 Tue 10:15 BEY/0127

Modeling resonant soliton interactions in the Kadomtsev-Petviashvili equation using PINNs — •Gerald Kämmerer — Universität Duisburg

Resonant two-soliton interactions in the Kadomtsev-Petviashvili (KP) equation are modeled using Physics-Informed Neural Networks (PINNs). This framework directly solves the KP equation by incorporating the governing partial differential equation residuals into the loss function, specifically focusing on Y-shaped resonances and web-like patterns that occur under specific resonance conditions. Comparisons with known algebraic solutions show a good agreement in capturing characteristic interaction patterns. To accelerate the learning of complex dynamics, progressive training strategies and symmetry-informed network architectures are implemented, embedding the equation's inherent coordinate symmetries. The results demonstrate that PINNs can capture the rich dynamics of resonant soliton interactions, offering a framework for exploring parameter regimes beyond traditional numerical methods.

AKPIK 2.5 Tue 10:30 BEY/0127

Phase Transitions reveal Accuracy Hierarchies in Deep Learning — •Ibrahim Talha Ersoy[1], Andrés Fernando Cardozo Licha[2], and Karoline Wiesner[1] — [1]Universität Potsdam, Institut für Astronomie und Physik, Potsdam, Deutschland — [2]Universidade Federal Fluminense, Instituto de Física, Niterói, Brazil

Training Deep Neural Networks relies on the model converging on a high-dimensional, non-convex loss landscape toward a good minimum. However, much of the phenomenology of training remains ill understood. We focus on three seemingly disparate phenomena: the observation of phase transitions akin to statistical physics, the ubiquity of saddle points, and mode connectivity which is key for the active research area of model merging. We bring these into a single explanatory framework, that of the geometry of the loss and error landscapes. We show analytically that phase transitions in DNN learning are governed by saddle points in the loss landscape. Furthermore, we present a simple, easy to implement and fast algorithm, using the L2 regularizer as a tool, to explore the geometry of error landscapes. We demonstrate its use for efficiently finding paths connecting global minima by confirming the mode connectivity for DNNs trained on the MNIST data set to then use it to show numerically that saddle points in DNN loss landscapes mark transitions between distinct models that encode distinct digits of the MNIST data. Our work establishes the geometric origin of key DNN training phenomena and reveals hierarchically ordered accuracy basins analogous to phases in statistical physics.

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

Time: Tuesday 11:00–12:45 Location: BEY/0127

AKPIK 3.1 Tue 11:00 BEY/0127

Agentic Exploration of Physics Models — •Maximilian Nägele[1,2] and Florian Marquardt[1,2] — [1]Max Planck Institute for the Science of Light — [2]FAU Erlangen

The process of scientific discovery relies on an interplay of observations, analysis, and hypothesis generation. Machine learning is increasingly being adopted to address individual aspects of this process. However, it remains an open challenge to fully automate the heuristic, iterative loop required to discover the laws of an unknown system by exploring it through experiments and analysis, without tailoring the approach to the specifics of a given task. Here, we introduce SciExplorer, an agent that leverages large language model tool-use capabilities to enable exploration of systems without any domain-specific blueprints, and apply it to physical systems that are initially unknown to the agent. We test SciExplorer on a broad set of models spanning mechanical dynamical systems, wave evolution, and quantum many-body physics. Despite using a minimal set of tools, primarily based on code execution, we observe impressive performance on tasks such as recovering equations of motion from observed dynamics and inferring Hamiltonians from expectation values. The demonstrated effectiveness of this setup opens the door towards similar scientific exploration in other domains, without the need for finetuning or task-specific instructions.

AKPIK 3.2 Tue 11:15 BEY/0127

Executable Manuscripts as Jupyter Notebooks: The Next Evolution in Scientific Publishing? — •Sebastian Rejman[1,2], Ina Vollmer[2], and Bert Marc Weckhuysen[2] — [1]Fritz-Haber-Institute of the Max-Planck-Society, Berlin, Germany — [2]Utrecht University, Utrecht, The Netherlands

The scientific paper as we know it today has remained largely unchanged for over a century. While color figures are now standard, and the supporting information contains more and more of the evidence, the manuscript itself remains a static pdf. The tools available to us, however, have drastically improved. Internet connections are faster, compute and storage are cheap, and high-level programming languages like Python make analysis automation accessible to the non-expert programmer.

Jupyter Notebooks, familiar to many students learning to program, allow to combine text with code and interactive figures. These notebooks, if used together with data repositories like OSF along with analysis code hosted on GitHub, allow for a transparent and reusable publication of research results. The reader can reproduce the analysis and figures at the push of the button, and easily re-purpose both analysis code and the underlying data - Paving the way for studies with large datasets in the field of chemistry and the natural sciences in general.

In this contribution, we demonstrate the executable version of our recent work on the role of external acidity in the cracking of plastics and provide practical guidance for implementation.

AKPIK 3.3 Tue 11:30 BEY/0127

PaperVerse: Disrupting the Peer-Review Process via AI-Driven Analysis and Reviewer Compensation — •Hendik Zobel, Oliver Mey, and René Stemmler — PaperVerse UG (haftungsbeschränkt), Dresden, Germany

The current scientific publishing model faces a systemic bottleneck: it relies on the uncompensated labor of volunteer researchers, resulting in significant delays and undervalued expertise. This talk introduces PaperVerse, a platform designed to disrupt this paradigm by treating peer review as valuable, billable work - supported by generative AI.

We propose a dual-layer architecture. First, our active AI Review Engine provides immediate, automated feedback on preprints (e.g., from arXiv) and private uploads, allowing authors to iteratively improve their manuscripts before submission. Second, and most critically, we outline our vision for a monetized marketplace that directly compensates human reviewers. By offloading structural and stylistic critique to AI, we free experts to focus on deep scientific validation, ensuring they are financially rewarded for their intellectual contribution.

We will discuss how AI-driven insights pave the way for this shift from volunteerism to a fair, incentivized economy. PaperVerse aims to establish a sustainable ecosystem where algorithmic efficiency meets human expertise, finally giving peer review the market value it deserves.

Invited Talk AKPIK 3.4 Tue 11:45 BEY/0127
Model-free training of optical neural networks based on multimode semiconductor lasers — •Anas Skalli[1], Satoshi Sunada[2], Mirko Goldmann[1], Marcin Gebski[3], Nasibeh Haghighi[4], Stephan Reitzenstein[4], James A. Lott[4], Tomasz Czyszanowski[3], and Daniel Brunner[1] — [1]FEMTO-ST Institute / Optics Department, CNRS & Université Marie et Louis Pasteur, 15B avenue des Montboucons, 25030 Besançon Cedex, France. — [2]Faculty of Mechanical Engineering, Institute of Science and Engineering, Kanazawa University, Kakuma-machi Kanazawa, Ishikawa 920 1192, Japan. — [3]nstitute of Physics, Lodz University of technology, Wólczańska 217/22190-005 Łódź, Poland — [4]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

In this work, we demonstrate a fully autonomous and parallel optical neural network (ONN) based on a multimode VCSEL architecture using off-the-shelf components. The system is scalable in both network size and inference bandwidth, paving the way toward GHz-level computing. Our ONN supports in-situ learning, making it closer to true autonomous operation. To unlock the full potential of our hardware, we develop and benchmark several hardware-compatible optimization algorithms, including SPSA and PEPG, demonstrating their suitability for physical systems with limited computational resources, and showing how algorithmic choices impact convergence speed, scalability, and energy cost. Our ONN outperforms both a linear hardware baseline and a digital linear classifier on the MNIST task.

Invited Talk AKPIK 3.5 Tue 12:15 BEY/0127
Virtual Reality Gamification for Photonics, AI and More — •Arash Rahimi-Iman — I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

Amazing mixed or virtual reality (XR/VR) tools can boost excitement for various science topics across age groups. VR-enhanced lectures can visually address topics such as photonics or artificial intelligence, illustrate what space travel or a visit to periodic lattices of solids might be like, allow learners to play with beams and particles to solve quests, and do much more.

Game-like exploration environments can support self-paced learning and collaborative training, including multiplayer modes. This not only brings immersion, but also interaction and fun. Moreover, VR worlds can help circumvent typical limitations of traditional labs, such as access, safety, or resources. They promote an extraordinary variety of designs and implementations, such as toy experiments mimicking, for instance, laser optics, quantum and nanophysics, and more.

Here, I present in VR one example of a digital learning environment enabled by powerful computer game engines like UE5. Like a lab-on-a-chip combining several laboratory functions on a single integrated circuit, hence on a chip, my VR analog "lab-in-a-chip" (the virtual lab world) could bring together different virtual experiments and learning scenarios, with user-group–oriented gamification making them more tangible for learners and non-experts.

AKPIK 4: Focus: Deep Learning in Electromagnetics Research

Time: Tuesday 14:00–15:30 Location: BEY/0127

Invited Talk AKPIK 4.1 Tue 14:00 BEY/0127
Beyond the Hype: Can AI Truly Transform Photonics? — •Mehdi K. Hedayati — Durham University, Department of Engineering, Durham DH1 3LE, UK

AI has become a powerful enabler in photonics, offering new routes for accelerated design and materials discovery beyond conventional trial-and-error approaches. In our group, we have demonstrated several AI-driven photonic design frameworks, with selected results experimentally verified in the laboratory. These include AI-assisted metasurface design enabling direct mapping between geometry and structural colour*allowing multiple colours from a single geometry under strain*as well as machine-learning models that capture nonlinear relationships in amorphous metamaterials, leading to proof-of-concept devices such as metasurface perfect reflectors. Yet, alongside these successes, the field is increasingly shaped by exaggeration and misplaced expectations. In reality, AI rarely delivers deployable photonic technologies; instead, it proposes candidate materials, geometries, or structures that must still be fabricated and validated experimentally. Fabrication yield, scalability, and limited characterization throughput therefore remain the dominant bottlenecks, causing progress to saturate at the experimental stage. In this talk, we will review the current state of the art of AI in photonics, examine where the field is heading in the near future, identify the key limitations we are likely to face, and discuss realistic pathways forward to better align AI-driven design with experimental reality.

Invited Talk AKPIK 4.2 Tue 14:30 BEY/0127
Machine–learning assisted design of metasurfaces — Lukas Mueller, Alexander Wolff, Janis Krieger, Steffen Klingel, Ralf Stemler, and •Marco Rahm — RPTU Kaiserslautern-Landau, Erwin-Schroedinger-Strasse, 67663 Kaiserslautern, Germany

We present several applications of machine-learning-assisted metasurface design. The first study focuses on maximizing the received signal power for two users positioned at different angles relative to a reconfigurable intelligent surface (RIS) operating at 27 GHz and 31 GHz. The RIS must function as a frequency-selective yet independently tunable beam steerer, making the optimization of the varactor bias voltages a challenging task. The optimized voltage matrices successfully steered beams at both frequencies over angles from 10° to 45°. In parallel, the work explores metasurface designs with independent control of reflection amplitude and phase using physics-informed machine learning. To significantly reduce training data requirements, a Temporal Coupled Mode (TCM) model was introduced to capture the dynamic tuning behavior using only four simulations instead of hundreds. Machine-learning models predict TCM parameters directly from the metasurface geometry, enabling fast optimization. Furthermore, transfer learning was applied to composite unit-cell design, achieving comparable accuracy with far fewer simulations than direct training.

AKPIK 4.3 Tue 15:00 BEY/0127
Optical Human Action Recognition - Less can be more? — •Maximilian Zier, Stefan Sinzinger, Kathy Lüdge, and Lina Jaurigue — Technische Universität Ilmenau, Ilmenau, Germany

Automated recognition of human actions is becoming more relevant due to applications in areas such as surveillance and autonomous driving. Modern neural networks achieve nearly perfect classification accuracies across various action datasets. However, they rely on complex feature extraction methods that lead to long training times and significant computational demands. Focusing on sustainability and efficiency, Reservoir computing systems aim to deliver similar performance combined with reduced computational effort by only training the output layer. An optically implemented reservoir offers the prospect of processing at the speed of light and nearly unlimited scalability due to inherent parallelism. In this contribution, we present results of a human action recognition task using a hybrid opto-electronic set-up based on [1]. In contrast to previous works, we forgo common preprocessing and feature extraction methods and use raw video data as input to the reservoir. Our system lags behind large neural networks in terms of classification accuracy, but has very low hardware requirements. Additionally, we reduce the length of the video sequences to one second, thereby using less input data to perform classification than previous works.

[1] Antonik, P., Marsal, N., Brunner, D. et al., Nat Mach Intell 1, 530-537 (2019)

AKPIK 4.4 Tue 15:15 BEY/0127
Loss-Minimized Incoherent Photonic Computing with Interferometer Networks — •Mingwei Yang[1,2], Konrad Tschernig[1,2], Felix Kübler[1], Okan Akyüz[1], Lennart Mannteuffel[1], Enrico Stoll[1], and Janik Wolters[1,2] — [1]Technical University of Berlin, Berlin, Germany. — [2]German

Aerospace Center (DLR), Berlin, Germany.

We present an algorithm for loss-minimized incoherent photonic multiplication of N-dimensional vectors with $N \times N$ matrices on standard Clements Mach-Zehnder interferometer (MZI) meshes [1]. By implementing arbitrary unitary transformations with incoherent light sources, the method avoids phase control and additional MZI blocks required by singular value decomposition in coherent schemes [2]. Optical energy per multiply and accumulate operation scales as $E = const$ in our approach, compared to $E \sim N$ in the crossbar architecture [3]. Experimentally, we implement a 4×4 photonic MVM and demonstrate an optical convolutional neural network for MNIST classification, achieving 28 correct predictions out of 31 images. Utilizing our loss-minimized architecture, we aim to reduce input intensity to the single photon regime to explore the limitations from shot noise.

[1] Clements, William R., et al. "Optimal design for universal multiport interferometers." Optica 3.12 (2016): 1460-1465.
[2] Shen, Yichen, et al. "Deep learning with coherent nanophotonic circuits." Nature photonics 11.7 (2017): 441-446.
[3] Feldmann, Johannes, et al. "Parallel convolutional processing using an integrated photonic tensor core." Nature 589.7840 (2021): 52-58.

AKPIK 5: Poster

Time: Thursday 15:00–16:30 Location: P5

AKPIK 5.1 Thu 15:00 P5

ARTIFICIAL INTELLIGENCE in the automotive industry — •Ilya Anufriev — Moscow, Russia

Modern automotive industry is a high-tech industry where production and management processes require constant improvement in efficiency and cost reduction. The use of robotic conveyors and artificial intelligence technologies allows for significant results in optimizing production processes, improving product quality, and reducing operational costs. The leading trends in the automotive industry include automation of production processes, data analysis and demand forecasting, product quality management, logistics and supply chain management, and decision support. I have developed a model for implementing artificial intelligence to optimize workflows within an automotive organization.

AKPIK 5.2 Thu 15:00 P5

Physics-based Reinforcement Learning for Balancing the Cart-Pole — •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 lateral 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. Training the multiple hidden layers of Deep Q-Networks, however, is computationally expensive and thereby energy-demanding. Replacing these hidden layers with an Echo State Network reduces training costs while maintaining performance [2]. Echo State Networks have been shown to be replaceable by physical systems [3]. We explore the potential of solving the Cart-Pole problem with a physics-based Echo State Network.

[1] V. Mnih et al., Nature 518, 529 (2015)
[2] I. Polonskiy, Bachelor Thesis, University of Duisburg-Essen (11/2024)
[3] K. Everschor-Sitte et al., Nature Reviews Physics 6, 455 (2024)

AKPIK 5.3 Thu 15:00 P5

Stereovision-based angle and depth estimation for terahertz layer measurements — •Tim Arniko Meinhold[1,2], Dmytro Kharik[1], Joshua Hennig[1,2], Mirco Kutas[1,2], Jens Klier[1,2], Georg von Freymann[1,2], and Daniel Molter[1] — [1]Department for Materials Characterization and Testing, Fraunhofer Institute for Industrial Mathematics ITWM, 67663 Kaiserslautern, Germany — [2]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

Terahertz systems can measure layer thicknesses with high precision in a fully contactless, non-destructive manner. However, reliable results require accurate alignment of the beam perpendicular to the surface, as even small angular deviations can affect the measurements. Many optical approaches still struggle to combine precision and real-time capability on demanding surfaces. Meanwhile, advances in stereo imaging and machine-learning methods provide a framework to support stable, interpretable measurement conditions.

Here, we report a compact stereovision-based setup within a framework that includes neural network-based approaches. Our goal is a practical and reliable method that delivers precise depth and angular information, which are expected to improve terahertz real-time thickness measurements.

AKPIK 5.4 Thu 15:00 P5

Exploring Reinforcement Learning for Particle Transport in the Presence of Inhomogeneities — •Finn Marten Boyer, Atreya Majumdar, and Karin Everschor-Sitte — University Duisburg-Essen, Duisburg, Germany

Classical transport theories typically assume homogeneous media, yet real materials often exhibit inhomogeneities that limit the applicability of such models. In particular, standard approaches like renormalization may fail when particles encounter defects whose characteristic energy scales are comparable to or larger than their kinetic energies. We investigate reinforcement learning as a data-driven framework for optimizing particle transport in strongly inhomogeneous environments. Our work indicates the potential of reinforcement-learning-based approaches for particle dynamics in more realistic and complex systems.

AKPIK 5.5 Thu 15:00 P5

Supporting Physical and Computational Biology with AI-Powered Multi-agent Model Generation — •Prerana Chandratre, Anjali Sharma, and Justin Bürger — TUD Dresden University of Technology, Dresden, Germany

Many open biological questions, from human embryogenesis to complex diseases like cancer, cannot be solved by experiments alone but require integration with biophysical and computational modeling. To address this, our group developed the software Morpheus (https://morpheus.gitlab.io/) which has become a widely used open-source platform (Starruß et al., 2014). Morpheus is based on a declarative modeling language, MorpheusML, and such models together with their biological context are collected in the MorpheusML model repository. Yet, creating MorpheusML models remains a barrier, especially for wet-lab researchers and students without programming expertise. To resolve this bottleneck, we are developing a model generation tool that uses a multi-agent workflow based on large-language models. Planned enhancements include a simulation-in-the-loop architecture enabling iterative, agent-driven model refinement and validation, expansion of the training dataset with model-text pairs from the MorpheusML model repository, and integration of automated validation and benchmarking metrics. The outcome will be the Morpheus.AI modeling assistant that enables robust generation of valid MorpheusML models from textual input sources, including PDF manuscripts. These AI-generated models will empower both research and education in physical and computational biology.

AKPIK 5.6 Thu 15:00 P5

Persistent Homology-Based Indicator of Orientational Ordering in Experimental Skyrmion Lattices — •Michiki Taniwaki[1,2], Thomas Winkler[1,3], Jan Rothörl[1], Raphael Gruber[1], Chiharu Mitsumata[4], Masato Kotsugi[2], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [2]Department of Materials Science and Technology, Tokyo University of Science, Niijuku 125-8585, Japan — [3]Institute of Molecules and Materials, Radboud University, Heyendaalseweg 135, 6525AJ Nijmegen, The Netherlands — [4]Graduate School of Pure and Applied Sciences, University of Tsukuba, Tenodai 305-8571, Japan

Skyrmions are chiral spin textures whose topological protection makes them apt for low-power memory and logic devices. In two dimensions, skyrmion lattices can undergo topological phase transitions[1]. A central challenge is to quantify the configurational order of skyrmion lattices and to construct appropriate indicators that are sensitive

to topological defects. Here we use persistent homology (PH), a method from topological data analysis, to characterize experimental two-dimensional skyrmion lattices. We define new scalar measures of translational and orientational order and compare them with the conventional measure of the ordering. Our approach captures the signatures of the softening of configurational order. These results demonstrate that PH provides a compact and robust indicator of the order and is well suited to the study of topological phase transitions. [1] R. Gruber et al., Nat. Nanotechnol. 20, 1405-1411 (2025).

AKPIK 5.7 Thu 15:00 P5

Hybrid Machine Learning Framework for Predicting Cycling-Induced Ageing in Lithium-Ion Batteries — •Sandhra Ganesh — University of Münster Institute of Physical Chemistry AK Heuer 48149 Münster, Germany

Predicting cyclical capacity fade is critical for assessing the long-term reliability and second-life potential of lithium-ion batteries. Traditional physics-based ageing models provide valuable interpretability but are often computationally expensive and depend on parameters that are difficult to obtain experimentally. Conversely, purely data-driven methods offer efficiency but typically struggle to generalise across operating conditions and lack physical grounding.This work proposes a hybrid modelling framework that integrates physics domain knowledge with deep learning to more accurately capture cycling-induced degradation. The framework incorporates physically meaningful feature extraction from voltage, capacity, and operational profiles, together with physics-guided constraints that ensure realistic degradation behaviour without requiring detailed mechanistic models. The approach aims to improve predictive accuracy, interpretability, and transferability across varying conditions and datasets. Its effectiveness will be evaluated through cross-condition generalisation studies and assessments of practical cycle-life prediction accuracy.

AKPIK 5.8 Thu 15:00 P5

Enabling high performance analog photonic computing using SFP transceivers — •Arvid Gansäuer[1], Mingwei Yang[1,2], Okan Akyüz[1,2], Lennart Mannteuffel[1], Felix Kübler[1], Konrad Tschernig[1], Enrico Stoll[1], and Janik Wolters[1,2] — [1]Technische Universität Berlin, Berlin, Germany — [2]Institute of Space Research, German Aerospace Center (DLR), Berlin, Germany

Photonic analog processors promise energy-efficient, parallel computing, specifically to tackle future machine learning and artificial intelligence (ML/AI) workloads. The fundamental mathematical operation of ML/AI computations, vector-matrix multiplication, is naturally suited to be performed in an optical setting [1]. However, many approaches utilize specialized, custom-made light sources and modulators to encode input vectors [1,2]. In this work we use commercial 1550 nm SFP transceivers to encode these vector inputs. We employ the incoherent excitation approach, which enables the use of light pulses generated by independent transceivers without any phase stabilization. To encode vector elements as incoherent light amplitudes, we generate sequences of 0- and 1-pulses within a time bin shorter than the integration time of the measuring photodiode. Using an FPGA, we achieve parallel transmission of photonic signals via 4 transceivers at $1.25\,\mathrm{GHz}/N$, where N is the number of intensity levels to approximate the analog signal. Thus, our approach enables the use of robust, readily available SFP-transceiver modules for high-performance analog photonic computing. [1] Y. Shen et al. Nat. Photon. 11, no. 7, p. 441 (2017), [2] J. Feldmann et al., Nature 589, no. 7840, p. 52 (2021).

AKPIK 5.9 Thu 15:00 P5

Understanding phase transitions in information processing systems using Geometric Thermodynamics — •Jonas Maximilian Müller, Ibrahim Talha Ersoy, and Karoline Wiesner — University of Potsdam

Phase transitions are well understood phenomena which arise in many fields of physics. Near the transition point very different systems show identical behaviour in accordance to their universality class. The framework of Geometric Thermodynamics allows for a more abstract approach to the transitions. We have shown, that neural networks undergo phase transitions related to accuracy hierarchies. However, the full extent of the analogy is unclear and there is no direct mapping of the critical phenomena described for DNNs to a thermodynamical framework. Luckily, both systems can at least locally be described using information geometry. In this study we characterise the transition phenomenology of well known thermodynamical systems using Geometric Thermodynamics. Using the Fisher metric we then construct a precise mapping between information processing systems, specifically DNNs, and thermodynamic systems in the proximity of the transition point. This mapping will in turn help us explore the full extent of the phase transition analogy for DNNs and better understand how they process information by leveraging the knowledge and techniques of Thermodynamics and Statistical Physics.

AKPIK 5.10 Thu 15:00 P5

Advancing Machine Learning Optimization of Chiral Photonic Metasurface: Comparative Study of Neural Network and Genetic Algorithm Approaches — •Davide Filippozzi[1], Alexandre Mayer[2], Nicolas Roy[2], Wei Fang[3], and Arash Rahimi-Iman[1] — [1]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University, Gießen, Germany — [2]Department of Physics, Namur Institute for Complex Systems (naXys), University of Namur, Belgium — [3]College of Optical Science and Engineering, Zhejiang University, Hangzhou, China

We report on an advanced optimization framework for chiral photonic metasurfaces, comparing a refined Neural Network (NN) pipeline against a Genetic Algorithm (GA). By introducing a two-output NN architecture and exploiting geometric symmetries for data augmentation, we successfully reduce the trade-off between circular dichroism (CD) and reflectivity. Our comparative analysis on GaP and PMMA structures reveals complementary strengths: the GA excels in finding global optima for complex geometries, while the NN provides superior computational efficiency for large-scale screening. The optimized designs demonstrate a close to twofold increase in CD compared to Ref. [Mey & Rahimi-Iman, PSS-RRL 16, 2100571 (2022)]. We propose a hybrid workflow combining both methods to accelerate the design of effective chiral mirrors for polarization-selective light-matter interaction studies.

AKPIK 5.11 Thu 15:00 P5

Machine Learning for Tip Enhanced Raman Spectroscopy — •Harshit Sethi, Orlando Silveira, and Adam Foster — Aalto University, Espoo, Finland

Tip Enhanced Raman Spectroscopy (TERS) provides nanoscale chemical fingerprint alongside high-resolution topographic mapping of molecules, offering a powerful tool for materials discovery. However, TERS image datasets are challenging to interpret and typically demand time-consuming, computationally intensive quantum*chemistry calculations. To overcome this problem, we present an encoder-decoder model trained and evaluated on simulated TERS images of planar molecules, enabling direct prediction of molecular structures from spectral simulated data with high accuracy. Our approach demonstrates the feasibility of automating molecular structure identification from TERS images, bypassing traditional manual analysis. These findings provide a foundation for extending machine learning methods to experimental TERS datasets, potentially accelerating molecular discovery by integrating nanoscale spectroscopy with automated computational analysis.

AKPIK 5.12 Thu 15:00 P5

Non-unitary time evolution via the Chebyshev expansion method — •Aron Hollo[1,2], Daniel Varjas[3,4,5], Cosma Fulga[3,4], Laszlo Oroszlany[1,2], and Viktor Konye[3,4,6] — [1]Department of Physics of Complex Systems, Eötvös Loránd University, Budapest, Hungary — [2]Wigner Research Centre for Physics, Budapest, Hungary — [3]Institute for Theoretical Solid State Physics, IFW Dresden, Dresden, Germany — [4]Würzburg-Dresden Cluster of Excellence ct.qmat, Germany — [5]Department of Theoretical Physics, Budapest University of Technology and Economics, Budapest, Hungary — [6]Institute for Theoretical Physics Amsterdam, University of Amsterdam, Amsterdam, The Netherlands

The Chebyshev expansion method is a highly efficient technique for computing the time evolution of quantum states in Hermitian systems with bounded spectra. In the physics literature, its applicability is often assumed to be restricted to real spectra within the interval [-1,1], limiting its use for non-Hermitian dynamics.

Here, we show that this restriction is not fundamental. The Chebyshev expansion of the exponential function remains mathematically valid over the entire complex plane and can therefore be applied to arbitrary non-Hermitian matrices. The apparent breakdown of the method outside the conventional spectral bounds is traced back to numerical rounding errors rather than to a failure of the expansion. By deriving an analytic upper bound for the accumulated rounding error, we obtain a practical criterion for selecting safe time steps based on

the spectral radius of the Hamiltonian.

AKPIK 5.13 Thu 15:00 P5

Nanomechanics-Driven Design of Flexible Textile-Based Metamaterials and Bio-Inspired Soft Composites — •Amine HAJ TAIEB — ISAMS, University of Sfax, Tunisia

Textiles, soft composites, and architectured metamaterials are emerging as key platforms for next-generation flexible systems in wearables, biomedical devices, adaptive structures, and energy-absorbing applications. Their unique mechanical performance*combining flexibility, stretchability, and durability*originates from complex interactions across multiple length scales, from fiber and yarn nanostructure to textile architecture and macroscopic response. Despite rapid progress, the lack of an integrated multiscale understanding still limits predictive design. This contribution explores how advanced nanomechanical characterization and multiscale modeling can accelerate the rational design of textile-based and bio-inspired flexible materials. Inspired by biological fibrous systems, we further discuss how hierarchical structuring and architectured textile geometries can be exploited to tune mechanical functionality. The integration of high-throughput testing and data-driven approaches, including machine learning, enables the identification of key design descriptors governing mechanical adaptability and robustness. By promoting interoperable experimental and simulation data, this work directly ontributes to a unified framework for the design of sustainable, high-performance textile-based flexible materials and metamaterial

AKPIK 5.14 Thu 15:00 P5

A Finite Element Homogenization Approach for Hollow Conductor Windings — •Shamim Aslam, Laura D'Angelo, and Herbert De Gersem — Institute for Accelerator Science and Electromagnetic Fields, TU Darmstadt, Germany

Future fast cycling synchrotrons require fast ramping dipole magnets. Due to high transients, eddy current and hysteresis effects become more pronounced in these magnets. Consequently, the associated thermal losses must be carefully considered in the overall magnet design. One key design solution to address this challenge is the use of hollow conductors. Hollow conductors facilitate the flow of electrical current while enabling efficient thermal cooling. Simulation-wise, hollow conductors are very challenging to compute as they impose a multi-scale problem, both geometrically and physically. The computational cost for multiscale geometries can be potentially reduced by using homogenization technique. We present an advanced homogenization technique for the simulation of hollow conductor windings, tackling this multi-scale problem while maintaining a sufficient accuracy. In this homogenization technique, the fine model containing hollow conductor windings replaced with a bulk region with equivalent material properties. As a validation of the homogenization technique, the method applied on a dipole magnet with 16 hollow conductors windings. This application example demonstrate the high accuracy, reduced computation time and easy implementation of our homogenization technique as compared with the brute force finite element simulations.

AKPIK 5.15 Thu 15:00 P5

Digital-Analog Simulations of Schrödinger Cat states in the Dicke-Ising Model — •Dmitrii Shapiro[1], Yannik Weber[1], Tim Bode[1], Frank K. Wilhelm[1,2], and Dmitry Bagrets[1,3] — [1]Quantum Computing Analytics (PGI-12), Forschungszentrum Jülich, Germany — [2]Saarland University, Germany — [3]University of Cologne, Germany

We study the Dicke-Ising model: an Ising chain where all spins couple to a common bosonic mode. Due to competing spin-spin and spin-boson interactions, the phase diagram exhibits both second- and first-order superradiant quantum phase transitions (QPTs). At the QPT, the system evolves into an entangled superradiant state with a boson condensate. We discuss the free-energy landscape near the QPT, obtained by integrating out the spins. We then propose a digital-analog quantum simulator for the Dicke-Ising Hamiltonian based on interacting qubits coupled to a single-mode resonator. The many-body propagator is decomposed via Trotterization into layers of single- and two-qubit rotations alternating with Jaynes-Cummings (JC) gates that emulate spin-boson coupling. The JC gate is analog, as it exploits rotations in the resonator's native Hilbert space. We show that the superradiant state can be approximated by a quench protocol with a finite-depth circuit. Applying a selective measurement of global qubit parity yields a Schrödinger cat state in the photonic subspace—a hallmark of the superradiant ground state in finite-size systems. The cat state can be probed via Wigner tomography of the resonator field. For details, see [Shapiro et al., PRA 112, 042412 (2025)].

AKPIK 6: AI Methods for Physics and Materials Science

Time: Thursday 16:45–18:30 Location: BEY/0127

AKPIK 6.1 Thu 16:45 BEY/0127

Recycling resources from aborted quantum key distribution protocols — •Siyuan Qi[1] and Ramona Wolf[2] — [1]Universität Siegen, Siegen, Germany — [2]Universität Siegen, Siegen, Germany

In quantum key distribution protocols, abortion often occurs due to detected errors or leakages. A secure protocol must ensure that if abortion does not occur, the generated key is secure. However, when abortion happens, the resources used are lost and cannot be reused, leading to waste. A malicious party, Eve, can exploit this by intentionally interfering with the protocol, forcing an abortion every time it's run. While Eve cannot obtain the secret key or avoid detection, she can prevent key generation and cause significant resource waste, which is undesirable in practical scenarios. This issue can be addressed by implementing procedures that recycle resources from aborted protocols or by preventing Eve from interfering in such a way. A protocol is aborted when the minimum entropy of the key generated does not exceed the leakage. If an abortion is caused by large leakage, we can still generate certified private randomness from the minimum entropy, provided it is not zero. Additionally, in specific scenarios where there is an identity designation process involved, we can move the identity designation to the last round so that Eve, not knowing she is a participant or not until the very end, will be discouraged from malicious behaviors.

AKPIK 6.2 Thu 17:00 BEY/0127

Causal–Physical Descriptor Discovery for Interpretable Materials Informatics — •Kanchan Sarkar and Axel Gross — Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany

Linking data-driven models to physically grounded behavior remains a key challenge in materials informatics. Data Nexus Vista (DNV1) is a causally informed framework that integrates domain knowledge with machine learning to identify interpretable descriptors. It provides standardized, configurable workflows spanning data preprocessing, feature construction, model training, and interpretation. DNV1 combines established feature-importance and descriptor-design tools with causal analyses, including counterfactual interventions, allowing for direct assessment of how model predictions respond to controlled changes. The framework supports both graphical and programmatic interfaces and provides descriptor-tracing utilities that map model features to physically meaningful variables. All workflows and outputs adhere to FAIR principles, ensuring reproducibility and transparency. The framework has been tested on multiple datasets and demonstrated with DFT-computed spinel cathodes. Rather than limiting ML models with fixed descriptors, DNV1 allows descriptors to emerge through causal interrogation of the data-physics nexus.

AKPIK 6.3 Thu 17:15 BEY/0127

Support for self-driving labs within the NOMAD ecosystem — •Sarthak Kapoor[1], Hampus Näsström[1], Ahmed Ilyas[1], Alvin N. Ladines[1], Alexander Fuchs[2], Joseph F. Rudzinski[1], Lauri Himanen[1], Sebastian Brückner[1], José A. Márquez[1], Martin Albrecht[3], and FAIRmat Team[1] — [1]Physics Department and CSMB, Humboldt-Universität zu Berlin, Germany — [2]Department Physik, FAU Erlangen-Nürnberg — [3]Department Materials Science, IKZ Berlin

Self-driving laboratories (SDLs) rely on robust digitization, structuring, and analysis of experimental data. We present NOMAD [nomad-lab.eu] [1] as a comprehensive research data management and workflow ecosystem that addresses the challenges inherent to emerging SDLs.

The NOMAD ecosystem supports direct interfacing with lab instruments and addresses the transformation of instrument outputs into machine-actionable formats, a key requirement in SDLs, through a flexible schema system that allows researchers to represent raw data as standardized entries based on community-developed or laboratory-specific definitions. NOMAD Actions provide a robust framework for defining, executing, and monitoring sophisticated analysis and decision-making SDL workflows, such as ML pipelines and Bayesian optimization strategies. Moreover, NOMAD's workflow storage framework facilitates detailed provenance tracking, along with tools for navigating workflow graphs. Together, these capabilities position NOMAD as a foundational toolkit for realizing scalable, reliable, and FAIR SDLs. [1] Scheidgen, M. et al., JOSS 8, 5388 (2023).

AKPIK 6.4 Thu 17:30 BEY/0127

Probabilistic greedy algorithm solver using magnetic tunneling junctions for traveling salesman problem — •Ran Zhang[1,2,3], Xiaohan Li[2], Caihua Wan[2,3,4], Raik Hoffmann[5], Meike Hindenberg[5], Yingqian Xu[2], Shiqiang Liu[2], Dehao Kong[2], Shilong Xiong[2], Shikun He[6], Alptekin Vardar[5], Qiang Dai[6], Junlu Gong[6], Yihui Sun[6], Zejie Zheng[6], Thomas Kämpfe[5,7], Guoqiang Yu[2,3,4], and Xiufeng Han[2,3,4] — [1]Present address: Max Planck Institute of Microstructure Physics, Halle (Saale), Germany — [2]Institute of Physics, Chinese Academy of Sciences, Beijing, China — [3]University of Chinese Academy of Sciences, Beijing, China — [4]Songshan Lake Materials Laboratory, Dongguan, China — [5]Fraunhofer IPMS, Dresden, Germany — [6]Zhejiang Hikstor Technology Co. Ltd, Hangzhou, China — [7]TU Braunschweig, Braunschweig, Germany

Combinatorial optimization is central to AI, logistics, and network design, yet classical methods often trade efficiency for solution quality. We introduce a probabilistic greedy solver that integrates spin-transfer-torque MTJ true random number generators with tunable switching statistics. A temperature parameter controls the balance between deterministic and stochastic choices. Applied to the traveling salesman problem, the framework achieves high-quality tours and surpasses simulated annealing and genetic algorithms in convergence speed, scalability, and computational cost.

AKPIK 6.5 Thu 17:45 BEY/0127

FAIR and Flexible Workflow Support within the NOMAD Infrastructure — •J.F. Rudzinski[1], T. Bereau[2], S. Botti[3], E.B. Boydas[1], N. Daelman[1], L. Himanen[1], S. Kapoor[1], A.N. Ladines[1], J.A. Márquez[1], B. Mohr[1], H. Näsström[1], and Fairmat Team[1] — [1]CSMB, HU Berlin — [2]ITP, Heidelberg Uni. — [3]RC-FEMS, Ruhr Uni. Bochum

NOMAD [nomad-lab.eu] [1, 2] is an open-source, community-driven research data infrastructure designed for modern physics. It provides FAIR-compliant storage, management, and analysis for diverse computational and experimental materials science data, and its modular, plugin-based architecture enables low-barrier extensions for adjacent and interdisciplinary domains. Here we present NOMAD*s workflow capabilities as a foundation for scalable and AI-ready data pipelines. A general workflow schema supports both standardized and custom workflows that record detailed provenance and link heterogeneous data streams. Standardized workflows enable powerful search, visualization, and automation features, while custom workflows support agile, project-specific digitalization. Workflow entries can be created via Python-based plugins, a YAML workflow specification, or the NOMAD ELN interface, ensuring accessibility for researchers with varying technical backgrounds. Combined with a toolkit for high-throughput interfacing, NOMAD provides a robust and sustainable digital infrastructure across physics subdisciplines.

[1] Scheidgen, M. *et al.*, JOSS **8**, 5388 (2023).
[2] Scheffler, M. *et al.*, Nature **604**, 635-642 (2022).

AKPIK 6.6 Thu 18:00 BEY/0127

Towards machine-learning-based on-the-fly analysis of neutron reflectometry — •Anne Rentzsch[1], Valentin Munteanu[1], Oliver Anyanor[2], Shreya Shah[1], Philipp Gutfreund[3], Rémi Perenon[3], Anthony Higgins[2], Vladimir Starostin[4], Alexander Hinderhofer[1], Dmitry Lapkin[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universistät Tübingen, 720726 Tügingen — [2]School of Engineering and Applied Science, Swansea University, Swansea SA1 8EN, Wales, United Kingdom — [3]Institut Laue-Langevin, 38000 Grenoble, France — [4]Cluster of Excellence 'Machine learning - new perspectives for science', Universität Tübingen, Maria-von-Linden-Straße 6, 72076 Tübingen, Germany

We present a real-time data analysis pipeline for neutron reflectometry that integrates `reflectorch`, a machine-learning-based software for reflectometry data analysis, into the IT infrastructure at the Institut Laue-Langevin. The workflow was tested during an experiment on the mixing behavior of bilayer thin films. Measured data are automatically reduced and analyzed, and the predicted sample parameters are returned to the instrument control system. The automated analysis can be triggered as frequently as every 10 seconds, enabling parameters and their uncertainties to be tracked with high temporal resolution and supporting continuous monitoring and data-driven adjustments. Compared to conventional software, `reflectorch` is up to two orders of magnitude faster. Together, these results pave the way for closed-loop experiments and demonstrate the potential of machine learning to enhance the efficiency of neutron reflectometry experiments.

AKPIK 6.7 Thu 18:15 BEY/0127

Multi-fidelity and -objective optimization of ONCV pseudopotentials — •Austin Zadoks[1], Cameron Hargreaves[2], Jusong Yu[1], Weiguo Jing[2], Matteo Giantomassi[2], Gian-Marco Rignanese[2], and Giovanni Pizzi[1] — [1]PSI Center for Scientific Computing, Theory and Data, 5232 Villigen PSI, Switzerland — [2]Institute of Condensed Matter and Nanosciences, UCLouvain, Louvain-la-Neuve, Belgium

The pseudopotential (PSP) approximation is essential to the tractability of many first-principles methods. However, it requires balancing the number of pseudized states, basis-set convergence, and accuracy w.r.t. all-electron (AE) results. One notable method for constructing soft, faithful, and widely-supported PSPs is the optimized norm-conserving Vanderbilt (ONCV) approach[1]. Various strategies have been proposed for generating meta-optimal tables of ONCVPSPs such as the SG-15[2], PseudoDojo[3], and SPMS[4]. Recent efforts to verify DFT codes have highlighted the importance of high-quality PSPs and expanded the necessary AE reference data, notably through $Z = 96$[5]. We present a fully-automated multi-fidelity multi-objective Bayesian optimization of ONCVPSPs targeting these reference data. This approach allows for the efficient mapping of the high-fidelity PW-DFT Pareto frontier by leveraging lower-fidelity intermediate radial- and PW-DFT results.

[1] D.R. Hamann. PRB, 88 (2013). [2] M. Schlipf & F. Gygi. Comp. Phys. Comms., 196 (2015). [3] M.J. van Setten, et al. Comp. Phys. Comms., 226 (2018). [4] M.F. Shojaei, et al. Comp. Phys. Comms., 283 (2023). [5] E. Bosoni, et al. Nat. Rev. Phys., 6 (2024).