

# 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	<b>3D Integration Towards Autonomous Optical Neural Networks</b> — •ADRIÀ GRABULOSA, ANAS SKALLI, DANIEL BRUNNER
AKPIK 4.1	Tue	14:00–14:30	H5	<b>The Scaling of Intelligence: From Transformers to Agentic AI</b> — •OLIVER MEY
AKPIK 4.2	Tue	14:30–15:00	H5	<b>Inverse Design in Electromagnetics with Artificial Intelligence</b> — •WILLIE PADILLA
AKPIK 4.3	Tue	15:00–15:30	H5	<b>Inverse design of lateral hybrid metasurfaces with machine learning</b> — •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	<b>Learning physically constrained microscopic interaction models of functional materials</b> — •BORIS KOZINSKY
SYMD 1.2	Mon	15:30–16:00	H1	<b>GRACE universal interatomic potential for materials discovery and design</b> — •RALF DRAUTZ
SYMD 1.3	Mon	16:00–16:30	H1	<b>Multiscale Modelling &amp; Machine Learning Algorithms for Catalyst Materials: Insights from the Oxygen Evolution Reaction</b> — •NONG ARTRITH
SYMD 1.4	Mon	16:45–17:15	H1	<b>Inverse Design of Materials</b> — •HONGBIN ZHANG
SYMD 1.5	Mon	17:15–17:45	H1	<b>Data-Driven Materials Science</b> — •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	<b>Predicting interaction partners and generating new protein sequences using protein language models</b> — •ANNE-FLORENCE BITBOL
SYAI 1.2	Thu	10:00–10:30	H1	<b>Realizing Schrödinger’s dream with AI-enabled molecular dynamics</b> — •ALEXANDRE TKATCHENKO
SYAI 1.3	Thu	10:30–11:00	H1	<b>Emergent behavior of artificial intelligence</b> — •STEFFEN RULANDS
SYAI 1.4	Thu	11:15–11:45	H1	<b>AI in medical research - navigating complexity with AI</b> — •DANIEL TRUHN
SYAI 1.5	Thu	11:45–12:15	H1	<b>Computational Modelling of Morphogenesis</b> — •DAGMAR IBER

#### Sessions

AKPIK 1.1–1.3	Sun	16:00–18:15	H2	<b>Hands-on Tutorial: AI Fundamentals for Research (joint session BP/TUT/DY/AKPIK)</b>
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AKPIK 2.1–2.4	Tue	9:30–10:30	H5	<b>Machine Learning Prediction and Optimization Tasks</b>
AKPIK 3.1–3.5	Tue	11:00–12:30	H5	<b>Research with AI: Hardware, Software, Tools</b>
AKPIK 4.1–4.3	Tue	14:00–15:30	H5	<b>Focus: Applications of Deep Neural Networks</b>
AKPIK 5.1–5.19	Thu	15:00–16:30	P2	<b>Poster</b>
AKPIK 6.1–6.6	Thu	16:30–18:00	H5	<b>AI Methods for Materials Science</b>