AI4MAT-ICLR-2026: ICLR 2026 WORKSHOP ON AI FOR ACCELERATED MATERIALS DESIGN

ABSTRACT

AI4Mat-ICLR-2026 explores the automated discovery of advanced materials through three interconnected pillars: 1. AI-Guided Design; 2. Automated Synthesis; 3. Automated Characterization. By bringing together leading researchers at the intersection of machine learning and materials science, the workshop fosters discussion of cutting-edge advances while building a cohesive, multidisciplinary community tackling some of the field's most pressing challenges. To that end AI4Mat-ICLR-2026's program highlights two leading topics to foster scientific dialogue in relevant subject areas, each featuring carefully curated invited speakers: 1. Reinforcement Learning & Beyond: The Role of Feedback in AI for Materials Science; 2. Cross-Modal, Unified Materials Representations – From Structure to Properties to Performance. In addition to invited talks and technical discussions, AI4Mat-ICLR-2026 continues its commitment to community development through established initiatives, including a Tiny Papers track for early-stage work, travel grants to support broad and inclusive researcher participation, and a dedicated journal venue for high-quality submissions.

1 INTRODUCTION

We propose a full-day, medium-sized workshop at ICLR 2026 titled "AI for Accelerated Materials Design" (AI4Mat-ICLR-2026). This workshop will serve as a venue for researchers at the intersection of AI and materials science to address pressing scientific challenges using AI-driven techniques, as illustrated in Figure 1. AI is presently transforming materials science and engineering, driving major global research initiatives from academic and government institutions (National Institute of Standards and Technology (NIST), 2024; University of Toronto, 2024; mol, 2023; Pennsylvania State University, 2024; National Science Foundation (NSF), 2024) and corporate research labs (IBM Research, 2024; Merck KGaA and Corporation, 2023; Microsoft Research, 2024; FAIR Chem, 2024), alongside the rise of several startups for AI driven materials discovery (Lohr, 2025; Metz, 2025; Radical AI, 2024; CuspAI, 2025; PhaseTree, 2024; Entalpic AI, 2024; Orbital Materials, 2024). To foster collaboration among these diverse stakeholders, our workshop will take an inclusive approach to materials design, encompassing a broad range of matter forms such as crystals, polymers, molecules, nano-materials, amorphous materials, and high-entropy materials. This holistic approach will ensure comprehensive discussions and foster novel directions across the materials landscape.

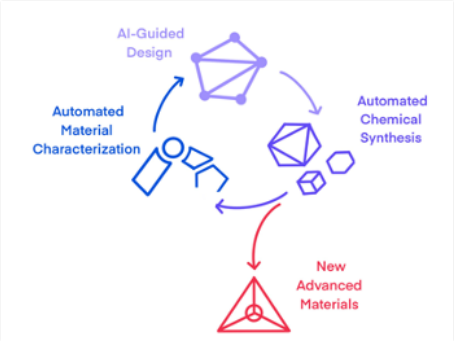

Figure 1: AI-Accelerated Materials Design leveraging 1) AI-Guided Design; 2) Automated Chemical Synthesis; and 3) Automated Material Characterization.

Drwaing on the success of previous AI4Mat workshops at NeurIPS (2022, 2023 & 2024) and ICLR (2025), as well as the upcoming AI4Mat-NeurIPS-2025 workshop, AI4Mat-ICLR-2026 aims to expand the workshop's reach to a broader audience and align with ICLR's focus on representation learning by fostering deep discussion on learning from diverse data modalities. AI4Mat-2022 (Miret et al., 2022) was the first NeurIPS workshop to take a comprehensive look at automated materials discovery spanning AI-guided design—mainly performed *in silico* using simulation tools—as well as automated chemical synthesis and automated material characterization. AI4Mat-2023 built upon the success of AI4Mat-2022 by focusing on how AI can accelerate the design of real-world materials experiments for synthesis and characterization. The workshop doubled its accepted submissions and introduced a travel grant program funded by corporate sponsors, enabling diverse student participation. Additionally, AI4Mat-2023 launched a themed collection with the Royal Society of Chemistry *Digital Discovery* journal (Miret et al., 2024). In 2024, the community expanded further

with two parallel workshops—AI4Mat-Vienna-2024 and AI4Mat-NeurIPS-2024—which provided forums for discussing the most pressing questions at the intersection of AI and materials science, along with a themed collection in Machine Learning Science and Technology (Miret et al., 2025). We are committed to expanding the AI4Mat initiative at ICLR-2026, building on the success of AI4Mat workshops at both ICLR-2025 and NeurIPS-2025. The strong alignment between our workshop's technical scope and ICLR's community positions us well to continue this growth.

AI4Mat-ICLR-2026 Technical Discussions: The goals of AI4Mat-ICLR-2026 focus on understanding two crucial and unique technical challenges that have emerged in AI for materials design:

1. Reinforcement Learning & Beyond: The Role of Feedback in AI for Materials Science:

Feedback-driven learning has demonstrated substantial promise across diverse AI applications, from robotics to large language models (Narayanan et al., 2025; Buehler, 2025; Tang et al., 2025; Guo et al., 2025). Materials science, however, presents unique challenges: experimental data is sparse, expensive to generate, and time-intensive to collect. Feedback-based approaches offer a compelling solution by creating iterative learning loops that integrate experimental outcomes, computational predictions, and expert knowledge (Tagasovska et al., 2024). By incorporating this multifaceted feedback, such approaches can accelerate discovery workflows and guide more efficient exploration of the vast materials space, enabling the development of novel compounds and systems.

2. Cross-Modal, Unified Materials Representations – From Structure to Properties to Performance:

AI4Mat-ICLR-2025 initiated a broader technical conversation on effective materials representations through its session "What are Next-Generation Representations of Materials Data?". While our previous session and related discussion focused primarily on developing specialized representations for specific problem settings, AI4Mat-ICLR-2026 expands the scope to address a more fundamental challenge: fusing and aligning multiple data modalities. Real-world materials systems generate diverse data types—structural characterization, property measurements, and performance metrics—each with distinct characteristics and requirements (Qu et al., 2024; Damewood et al., 2023). Meaningful insights, however, emerge only through unified understanding across these modalities. This session examines cutting-edge methods for integrating heterogeneous materials data sources into comprehensive predictive models that capture the full complexity of materials behavior. We will explore current approaches and open challenges in creating such integrated representations, with the goal of enabling frameworks that can reliably predict and optimize materials performance in practical applications.

AI4Mat-ICLR-2026 Community Building: AI4Mat has taken deliberate steps to cultivate an inclusive, interdisciplinary research community at the intersection of AI and materials science. We are committed to creating venues that both amplify high-quality research and welcome diverse perspectives from researchers across the globe. AI4Mat-ICLR-2026 represents a pivotal opportunity for community growth as the first AI4Mat workshop hosted in Latin America. This location enables us to meaningfully expand participation from historically underrepresented regions, particularly South and Central America. Previous workshops have drawn strong participation from North America, Europe, and East Asia. AI4Mat-ICLR-2025 enabled us to grow our representation from Southeast Asia and the Middle East, and we hope that AI4Mat-ICLR-2026's location in Brazil will allow us to deepen engagement with South and Central American research communities and foster new collaborations. To continue building an inclusive AI4Mat community, facilitate discussions on critical technical challenges, and strengthen networking opportunities, we plan to leverage:

1. Travel Grant Program: Building upon the accomplishments of prior AI4Mat NeurIPS and ICLR workshops, we plan to continue the travel grant program funded by AI4Mat corporate sponsors. Past years' successes have shown us that the travel program enables the participation of diverse, junior researchers who otherwise would not have the financial means to attend. AI4Mat-ICLR-2026 would provide a unique opportunity to encourage participation from geographically closer regions in South and Central America through travel grants, who have historically been underrepresented.

2. Tiny Papers Track: Building on the achievements of AI4Mat-ICLR-2025 and the ICLR Tiny Papers track, we plan to create a specific track for 2-page extended abstract to encourage broader participation. This extends our efforts in supporting inclusive research participation through our Findings track at prior AI4Mat workshops, where we encourage researchers

to submit often overlooked research efforts, such as engineering challenges and negative results.

3. Themed Submission Track - Feedback-Based Learning for Materials Design: Themed submission tracks have proven effective at generating productive ideas and discussion from the research community. This year, we are aligning our themed track with one of the panel sessions and will invite authors of high-quality papers to engage directly with invited speakers. We plan to select a small number of spotlight authors for a dedicated panel discussion, fostering conversation around practical challenges in feedback-based learning for materials science.
4. Journal Track: We aim to build on the success of AI4Mat-2023's, AI4Mat-NeurIPS-2024's and AI4Mat-ICLR-2025's journal track (Miret et al., 2024; 2025) to provide AI4Mat researchers the opportunity to submit their work to a prestigious venue for wider recognition.

AI4Mat's Interdisciplinary Research: The interdisciplinary research showcased at AI4Mat-ICLR-2026 reflects a rapidly maturing field at the convergence of AI and materials science. This growth is evident across multiple dimensions: a sharp increase in published research (Butler et al., 2024), the emergence of complementary workshops exploring various facets of this intersection (Wang et al., 2023; Regev et al., 2024), substantial institutional investments spanning large-scale academic research institutes (National Institute of Standards and Technology (NIST), 2024; University of Toronto, 2024; mol, 2023; Pennsylvania State University, 2024; National Science Foundation (NSF), 2024), continued industrial R&D efforts (IBM Research, 2024; Merck KGaA and Corporation, 2023; Microsoft Research, 2024; FAIR Chem, 2024), and a wave of specialized startups (Lohr, 2025; Metz, 2025; Radical AI, 2024; CuspAI, 2025; PhaseTree, 2024; Entalpic AI, 2024; Orbital Materials, 2024). Moreover, AI4Mat naturally aligns with diverse research areas already central to ICLR, many of which have been featured in past AI4Mat workshops. These include representation learning for materials modeling, generative methods for materials discovery, geometric deep learning, robotic learning for chemical synthesis, and multi-modal machine learning for materials characterization, to name a few.

AI4Mat's Unique Perspective & Distinction from Other ICLR Workshop

AI4Mat's unique value lies in bridging two communities with complementary expertise: materials scientists who understand critical domain challenges and the ICLR community with deep strengths in cutting-edge AI techniques. This targeted interdisciplinary approach has consistently fostered substantive technical exchanges, drawing speakers, submissions, and attendees from both fields across diverse institutions. By focusing specifically on impactful materials science problems that can be addressed through novel machine learning methods, AI4Mat occupies a unique position among workshops at major ML conferences. Specifically, while related workshops at ICLR, ICML, and NeurIPS have explored ML for molecules and computational materials modeling (Regev et al., 2024; Wang et al., 2023), drug discovery (Uehara et al., 2024), and synthetic biology (Liu et al., 2024; NaderiAlizadeh et al., 2024)—often emphasizing predictive or generative algorithms—AI4Mat takes a broader systems perspective. We focus on the end-to-end scientific workflow for creating new materials, including the automation of real-world experiments at each stage of the discovery process. This holistic view encompasses not only computational prediction and generation, but also experimental design, robotic synthesis, characterization, and the integration of these components into cohesive automated pipelines. Similarly, while workshops at the broad intersection of AI and physical sciences (Maskey et al., 2024; Maddix et al., 2024; Chen et al., 2024; Hartman et al., 2024; Welling et al., 2024) provide valuable forums for cross-domain discussion, AI4Mat maintains a sharper focus on materials design challenges. This specificity enables deeper engagement with domain-specific technical problems while remaining complementary to broader AI-for-science discussions.

2 AI4Mat-ICLR-2026 Proposed Workshop

AI4Mat-ICLR-2026 brings together leading AI and materials science experts representing diverse technical perspectives, career stages, institutional types, and geographic regions. Our organizing committee and invited speakers span industry labs, academic institutions, and startups from across the globe, reflecting our commitment to inclusive, multi-perspective dialogue. This diversity has proven essential to the substantive technical discussions that characterized previous AI4Mat workshops at NeurIPS and ICLR, and remains central to our dual goals of advancing technical innovation and broadening community participation. Given the increased volume of research relevant to AI4Mat, **we**

Table 1: Proposed AI4Mat-ICLR-2026 workshop schedule including invited speakers with **confirmed speakers** highlighted in bold. The workshop includes structured discussion time, a poster session, as well as substantial time for informal networking. We focus on bringing technical leaders from diverse institutions, seniority, and background to foster deep technical discussions with the AI4Mat audience.

Timeslot	Description	Participants
8.00-8.15	Opening Remarks	*Workshop Committee*
8.15 - 9.25	Talks Reinforcement Learning & Beyond: The Role of Feedback in AI for Materials Science?	*Workshop Committee & Invited Speakers* **Heng Ji** - Professor, University of Illinois, Urbana-Champaign **Andrew Beam** - Chief Technology Officer, Lila Sciences **Kyunghyun Cho** - Exec. Director of Frontier Research - Genentech Research
9.25 - 10.00	Interactive Panel Reinforcement Learning & Beyond	*Invited Speakers & AI4Mat Paper Authors* Drawn from Invited Speakers & Workshop Submissions
10.00 - 10.30	Coffee Break & Networking Tables	*Everyone*
10.30 - 12.00	Spotlights Session	Drawn from Workshop Submissions
12.00 - 13.30	Lunch & Poster Session	*Everyone*
13.30 - 15.00	Talks + Panel Cross-Modal, Unified Materials Representations From Structure to Properties to Performance	*Workshop Committee & Invited Speakers* **Xiaonan Wang** - Professor, Tsinghua University **Pascal Friedrich** - Professor, Karlsruhe Institute of Technology Pilar Cossio - Research Scientist & Project Leader, Flatiron Institute
15.00 - 15.30	Coffee Break & Networking Tables	*Everyone*
15.30 - 16.30	Spotlights Session for *Reinforcement Learning & Beyond*	Drawn from Workshop Submissions
16.30 - 17.00	Spotlights Session	Drawn from Workshop Submissions
17.00 - 17.15	Closing Remarks & Travel Grant Awards	*Workshop Committee*

expect a medium-sized attendance of $\sim$170 people at AI4Mat-ICLR-2026, which we believe will be conducive to deep technical exchange and networking.

2.1 AI4MAT NEURIPS WORKSHOPS & AI4MAT-ICLR-2025

AI4Mat-ICLR-2026 builds strategically on insights from previous workshops, incorporating both their successes and lessons learned. Our approach emphasizes deep technical discussions on unique AI-materials challenges, focuses on timely questions given the field's rapid evolution as well as alignment with the theme of the event, such as cross-modal representation learning, and prioritizes inclusive community building with expanded geographical and demographic representation.

AI4Mat-NeurIPS-2022 established the foundation with 40 accepted papers (including 12 spotlights) spanning all three research themes and $\sim 60-70$ participants. The program primarily featured lecture-style presentations introducing the latest progress in AI-Guided Design, Automated Chemical Synthesis, and Automated Material Characterization. AI4Mat-NeurIPS-2023 doubled in scale with 80 accepted papers and 15 spotlights, attracting ~ 120 participants. Learning from the inaugural workshop, we expanded the program format to address real-world materials challenges through Sim2Mat Lightning Talks and a dedicated panel, while exploring the emerging role of LLMs via a Fireside Chat on LLMs for Materials Design. Relevant insights from these discussions were documented in an openly available perspective article (Miret et al., 2024). AI4Mat-NeurIPS-2024 included 78 accepted papers (including 14 spotlights) with greater community participation of $\sim 200-250$ people. AI4Mat-NeurIPS-2024 tackled critical questions around creating real-world materials systems at global scale and integrating AI with physical experiments. Discussions yielded actionable insights on data creation, experimental reproducibility, new market exploration, and scaling existing materials applications (Miret et al., 2025). AI4Mat-ICLR-2025 included 66 accepted papers (including 14 spotlights) with strong community showing of ~ 150 people, including broader geographical participation. AI4Mat-ICLR-2025 included valuable scientific discussions on processing data from real-world materials experiments, along with introducing new ideas for materials representations. AI4Mat-NeurIPS-2025, which will be held later this year, has 115 accepted paper showing increasing interest in this research area.

3 DIVERSITY STATEMENT

We have assembled a diverse team of speakers and organizers whose varied perspectives and expertise will advance both the technical depth and community-building mission of AI4Mat-ICLR-2026. Our speaker lineup represents diversity across multiple dimensions: gender (3 women, 3 men), ethnicity, institutional type (3 academic, 2 industry, 1 non-profit research institute), and career stage (ranging from university faculty to corporate leadership and government researchers). This breadth ensures multifaceted discussions that address challenges from research, industrial, and policy perspectives. Our committee spans diverse geographies, genders, ethnicities, career stages, and underrepresented identities, bringing essential perspectives to workshop planning and execution. We continue expanding our PC with global representation across 40+ institutions spanning North and South America, Europe, East Asia, South Asia, and the Middle East. This geographical diversity ensures review processes that recognize varied research contexts and methodologies.

Inclusive Participation: We will craft our call for submissions to explicitly welcome contributions from researchers with diverse demographic and technical backgrounds across all tracks, including the Tiny Papers track designed to lower barriers to participation. Our themed submission tracks will facilitate informal mentoring by focusing discussions around concrete technical challenges, encouraging knowledge exchange and fostering new collaborations among participants at different career stages. By embedding diversity and inclusion at every level—from speakers to reviewers to participants—we aim to create an environment where varied perspectives drive innovation and where all community members feel empowered to contribute.

4 LOGISTICS & IMPLEMENTATION

We will record all presentations (live or pre-recorded), including accepted spotlights and invited speakers, and make them available online to maximize accessibility and broader community reach. The website will provide submission guidelines, including our LLM usage policy, along with information on workshop goals and organizers. To grow the community and encourage diverse sets of submissions, we will maintain the successful submission categories from past AI4Mat workshops (Papers, Tools & Findings, Tiny Papers, and a themed track) while jointly conducting targeted outreach. This approach encourages a broad range of technical work, particularly on the experimental materials side, which advances the state-of-the-art and fosters discussion among researchers. For review, we will use OpenReview, which automatically manages conflicts of interest, and require at least three reviewers per submission. To ensure consistency, we will publish reviewing criteria on the workshop website in advance, making them available to both authors and reviewers. All accepted submissions will be made publicly available on the website, continuing our practice from past AI4Mat workshops.

4.1 TIMELINE

- ICLR Decision & Website Update: December 1, 2025 & December 28, 2025
- Submission Deadline & Notification: February 1, 2026 & March 1, 2026
- Workshop: April 26 or April 27, 2026

Workshop URL: `https://sites.google.com/view/ai4mat`

INVITED SPEAKERS

Our invited speakers will share their insights on the major themes of AI4Mat-ICLR-2026 and were chosen to represent both the technical depth and growing diversity of the research community working at the intersection of AI and materials science.

Heng Ji - University of Illinois at Urbana-Champaign- Google Scholar Website Heng Ji is a Professor and Associate Head of Research at the Siebel School of Computing and Data Science at the University of Illinois Urbana-Champaign. She is an Amazon Scholar and serves as Founding Director of the Amazon-Illinois Center on AI for Interactive Conversational Experiences (AICE). Professor Ji received her B.A. and M.A. in Computational Linguistics from Tsinghua University, and her M.S. and Ph.D. in Computer Science from New York University. Her research focuses on natural language processing, particularly information extraction, knowledge base population, and multilingual AI systems. Her numerous awards include the NSF CAREER Award (2009), Google Research Awards

(2009, 2014), IBM Watson Faculty Award (2012), and recognition as one of "AI's 10 to Watch" by IEEE Intelligent Systems in 2013. She received an Outstanding Paper Award at NAACL 2024 for work on extending the context length capabilities of large language models. Professor Ji's work has made foundational contributions to advancing AI systems' ability to understand and process natural language across multiple languages and modalities.

Heng's work on language, reinforcement learning along with recent research in materials science make her an excellent fit for Reinforcement Learning & Beyond: The Role of Feedback in AI for Materials Science.

Andrew Beam - Lila Sciences - Google Scholar Website Andrew Beam is Chief Technology Officer at Lila Sciences and Associate Professor of Epidemiology at the Harvard T.H. Chan School of Public Health. At Lila Sciences, Dr. Beam is helping build the world's first scientific superintelligence platform, which integrates AI models with autonomous laboratories to accelerate discovery across life, chemical, and materials sciences. Under his technical leadership, Lila recently raised a 235M Series A to expand its AI Science Factory platform that automates the entire scientific method—from experiment design and execution to observation and redesign. Prior to joining Lila as CTO, Dr. Beam served as a Senior Fellow at Flagship Pioneering, where he led machine learning activities across Flagship-backed companies. His expertise spans machine learning for biology and medicine, with particular focus on developing AI methods that can autonomously drive scientific discovery at unprecedented scale and speed.

Andrew's record on using feedback based mechanisms for real-world applications make him a great fit for Reinforcement Learning & Beyond: The Role of Feedback in AI for Materials Science.

Kyunghyun Cho - Prescient Design (Genentech) - Google Scholar Website Kyunghyun Cho is Co-Founder and Executive Director of Frontier Research at Prescient Design within Genentech Research & Early Development (gRED), where he leads AI-powered drug discovery and computational biology research. Previously, he served as a Research Scientist at Facebook AI Research from 2017 to 2020, contributing to foundational work in artificial intelligence and machine learning. His industry experience demonstrates a strong track record of bridging academic research with practical applications, particularly in leveraging deep learning to accelerate scientific discovery. His industry work complements his academic role as Glen de Vries Professor of Health Statistics and Professor of Computer Science and Data Science at New York University, where he co-directs the Global Frontier AI Lab alongside Yann LeCun.

Kyunghyun's record on using feedback based mechanisms for real-world applications in Prescient Design make him a great fit for Reinforcement Learning & Beyond: The Role of Feedback in AI for Materials Science.

Xiaonan Wang - Tsinghua Unviersity - Google Scholar Xiaonan Wang is an Associate Professor in the Department of Chemical Engineering at Tsinghua University, where she leads the Smart Systems Engineering research group. Her research focuses on developing intelligent computational methods for advanced materials discovery, combining multi-scale modeling, optimization, data analytics, and machine learning to enable smart and sustainable development. Professor Wang's work bridges computational chemistry, materials science, and artificial intelligence, with particular emphasis on applying AI and machine learning techniques to accelerate the design and discovery of polymers, nanomaterials, and other functional materials. Her research has contributed to advancing reinforcement learning methods for polymer generation and optimization of nanoparticle synthesis through machine learning approaches. She applies these computational methods to address challenges in advanced materials, energy systems, environmental applications, and sustainable manufacturing, demonstrating the powerful synergy between AI and materials engineering for real-world applications.

Xiaonan's work on machine learning and real-world materials applications make her an excellent fit for Cross-Modal, Unified Materials Representations – From Structure to Properties to Performance.

Pascal Friedrich - Karlsruhe Institute of Technology - Google Scholar Website Pascal Friederich is a Tenure-Track Professor at the Karlsruhe Institute of Technology (KIT), where he leads the AiMat research group focusing on artificial intelligence and machine learning for materials science and chemistry. His lab develops algorithms for decision making in autonomous labora-

tories, as well as machine learning methods for accelerated materials simulations and materials design. Professor Friederich's research combines quantum mechanical methods such as density functional theory with machine learning techniques, focusing on computational design of organic semiconductors and functional materials. His work spans graph neural networks, computational chemistry, and multiscale modeling to accelerate materials discovery. In 2022, Professor Friederich received the Heinz Maier-Leibnitz Prize from the German Research Foundation (DFG), the most important recognition for early-career researchers in Germany. Most recently, he was awarded the Manfred-Fuchs-Prize 2025 by the Heidelberg Academy of Sciences for his pioneering contributions to using AI in developing novel chemical materials, particularly for solar energy applications.

Pascal's long track record on machine learning research for materials, including molecules and solid-state materials, make him a great fit for Cross-Modal, Unified Materials Representations – From Structure to Properties to Performance.

Pilar Cossio - Flatiron Institute Google Scholar Website Pilar Cossio is a research scientist and project leader for Structural and Molecular Biophysics at the Flatiron Institute's Center for Computational Mathematics, a position she has held since April 2021. She earned her B.S. in Physics from the University of Antioquia in Colombia and her Ph.D. in Physics and Chemistry of Biological Systems from the International School for Advanced Studies (SISSA) in Italy. Before joining the Flatiron Institute, Cossio was a Max Planck Tandem Group Leader affiliated with both the University of Antioquia and the Max Planck Institute of Biophysics, and held postdoctoral positions at the National Institute of Health and the Max Planck Institute of Biophysics. Her research focuses on developing mathematical and computational methods to characterize protein structures and dynamics by integrating data from multiple experimental modalities—including cryo-electron microscopy, single-molecule force spectroscopy, and biomolecular simulations. A key innovation in her work is the application of simulation-based inference (SBI), a framework that combines physics-based simulators, statistical inference, and machine learning to analyze multi-modal biophysical experiments. This approach addresses the challenge of extracting molecular details from noisy experimental data by coupling deep learning models with physics-informed simulations, enabling researchers to move beyond traditional single-experiment analysis and integrate information across different measurement techniques. Her recent work includes developing methods for template matching and conformational modeling from cryo-EM data using deep generative models and active learning approaches.

Pilar's focus on using machine learning across multiple modalities to solve challenging problems in materials and chemistry, make her a great fit for Cross-Modal, Unified Materials Representations – From Structure to Properties to Performance.

ORGANIZERS

Our organizational team, profiled below, is well-suited to conduct this workshop, given both the diversity of our disciplines and our shared research interests in AI for accelerated materials design across diverse domains. Our team consists of researchers that have prior experience in both fields, have a varied set of affiliations, and hold various levels of seniority, all of which provide a diverse set of perspectives in the workshop organization process. Furthermore, our team includes committee members with past experience in organizing AI4Mat and other machine learning workshops, as well as committee members who are organizing for the first time, further strengthening our mix of perspectives. The broad institutional diversity of the organizing and program committees also enables us to effectively manage conflicts of interest in assessing the quality of workshop submissions.

Santiago Miret - Lila Sciences -Google Scholar - LinkedIn Santiago Miret is a Director of Machine Learning for Materials at Lila Sciences, where he focuses on research at the intersection of AI and materials science. His work builds on his past research experience at Intel Labs and his Ph.D. work in Materials Science and Engineering at UC Berkeley. Santiago's AI research efforts include generative models, reinforcement learning, graph neural networks, geometric deep learning, natural language processing and evolutionary algorithms. Santiago also has prior experience in organizing workshops and conferences spanning diverse institutions from academia, industry, government, and the general public. Santiago was an organizing committee member for AI4Mat-NeurIPS-2022, AI4Mat-NeurIPS-2023 and AI4Mat-NeurIPS-2024, AI4Mat-NeurIPS-2025, and AI4Mat-ICLR-2025.

Defne Circi - Duke University - Google Scholar - Website Defne Circi is a Ph.D. candidate in Mechanical Engineering and Materials Science at Duke University, advised by Professor Cate Brinson. She is also pursuing a concurrent master's degree in Computer Science and is part of the AI for Materials Understanding and Design (aiM) program. Her research focuses on applying multimodal large language models to scientific knowledge extraction, with an emphasis on extracting complex information from diverse data sources such as charts, tables, and text in materials science literature. Her work aims to automate insight extraction from scientific articles at scale and to build comprehensive knowledge graphs and databases that accelerate materials discovery. Previously, Defne completed internships at IBM Research and HZDR. Defne has (co-)organized multiple hackathons and seminar series, including the aiM Program seminar series and the global large language model hackathon in chemistry and materials. **Defne is a new organizer for AI4Mat-ICLR-2026.**

N. M. Anoop Krishnan - Indian Institute of Technology Delhi - Google Scholar - Website N. M. Anoop Krishnan is an Associate Professor in the Department of Civil Engineering jointly with the Yardi School of Artificial Intelligence at IIT Delhi. His research focuses on artificial intelligence and physics-based simulations for accelerated materials modeling and discovery, especially in the areas of graph neural networks, molecular simulations, multiscale modeling, and natural language processing. He has organized several symposiums and workshops in international conferences such as Materials Research Society (Fall 2020, 2021, 2022, 2023 and Spring 2021, 2022, 2023), the American Ceramic Society (GOMD 2019, 2020, 2021, 2022, 2023, 2024, 2025), Materials Science and Technology (MST 2019, 2020, 2021, 2022, 2023, 2024, 2025), Engineering Mechanics Institute (2019), to name a few. Anoop has received several awards, including the Humboldt Fellowship for experienced researchers (2023), Google Research Scholar Award (2023), the W. A. Weyl International Glass Science Award by the International Commission on Glass (2022), and the Young Associate by the Indian Academy of Sciences (2022). Anoop was an organizing committee member for AI4Mat-NeurIPS-2023, AI4Mat-NeurIPS-2024, AI4Mat-ICLR-2025, and AI4Mat-NeurIPS-2025.

Emily Jin - University of Oxford - Google Scholar - Website Emily is a PhD student in Computer Science at the University of Oxford and AstraZeneca working with Michael Brostein and İsmail Ceylan under a UKRI EPSRC Studentship. Her research interests include applying graph machine learning methods to challenges in drug discovery, such as target identification, molecular generation, and organic crystal structure prediction. Previously, Emily worked full time at Facebook (now Meta), and completed internships at Microsoft Research's Health Futures team and Merck KGaA's AI and Digital Health team. She also served as the former Vice President of the Oxford Women in Computer Science society and has experience organizing large events, such as the Oxbridge Women in Computer Science Conference and several other panels and talks across both industry and academia. Emily is also an organizer for the Learning on Graphs and Geometry seminar series at Oxford, which has over 150 subscribers. Emily is an organizer for AI4Mat-NeurIPS-2025 and a new organizer for AI4Mat-ICLR-2026.

Mohamad Moosavi - University of Toronto & Vector Institute & Acceleration Consoritum - Google Scholar - Website Mohamad Moosavi is an Assistant Professor of Chemical Engineering and Applied Chemistry at the University of Toronto, faculty member at the Vector Institute and the Acceleration Consortium, and a member of the NVIDIA Researcher Advisory Council on Physics Machine Learning and Climate Science. Mohamad directs the Artificial Intelligence for Chemical Science (AI4ChemS) research group, focusing on leveraging AI and computational methods for the discovery of advanced materials, with a focus on technologies related to energy and sustainability. Mohamad has (co-)organized multiple hackathons, symposiums, and seminar series, including the Acceleration Consortium seminar series and the large language model hackathon in chemistry and materials 2024 with more than 500 attendees globally. Mohamad was also an organizer for AI4Mat-ICLR-2025.

Stefano Martiniani - New York University - Google Scholar - Website Stefano Martiniani is an Assistant Professor of Physics, Chemistry, Mathematics at New York University. His research focuses on the development and application of optimization, sampling, and machine learning approaches to engineer function in biological and materials systems. He leads complex scientific software projects related to data standards, databases, and machine learning frameworks: He is the ML Lead for ColabFit, the largest public database of materials and chemical data specialized for training machine

learning interatomic potentials, and the lead PI of the FERMat project, a multi-institutional effort in collaboration with Amazon Web Services to develop foundation models for materials and chemical property prediction. He has experience organizing workshops, including at the American Physical Society annual (March) meeting, as well as AI4Mat-NeurIPS-2024. He is a co-founder of the *KIM Review* journal. His awards include the 2023 Interdisciplinary Early Career Scientist Prize from the International Union of Pure and Applied Physics (IUPAP), CZI Neuroscience Pair Pilot Project Award, Simons Foundation Faculty Fellowship, and the Outstanding Ph.D. Thesis Award from the University of Cambridge.

Program Committee We plan to increase the size of the program committee to manage the anticipated increase in number of submissions. Confirmed PC members indicated by checkmark (✓):

Abhishek Bagusetty, Aikaterini Vriza, Alankar Alankar (✓), Alex Hernandez-Garcia (✓), Alexandre AGM Duval (✓), Alston Lo (✓), Amit Gupta (✓), Amol Thakkar, Amuthan A Ramabathiran (✓), Andres Bran (✓), Angel Yanguas-Gil (✓), Anirban Chandra (✓), Anoop Krishnan (✓), Austin Henry Cheng (✓), Ayush Jain (✓), Bang Liu (✓), Carmelo Gonzales (✓), Cheng-Hao Liu (✓), Chenqing Hua (✓), Chenyang Li, Dana O-Connor, Daniel Cassar (✓), Daniel P. Tabor (✓), Daniel Levy (✓), Defne Circi (✓), Dorina Weichert, Edward Kim (✓), Elton Pan (✓), Evgeny Burnaev (✓), Emma Granqvist (✓), Emmanuel Bengio (✓), Eric Fuenmueller (✓), Emily Jin (✓), Fadwa El Mellouhi, Farzaneh Jalalypour (✓), Felix Strieth-Kalthoff (✓), Felix Therrien (✓), Flaviu Cipcigan (✓), Gary Tom (✓), Geemi Wellawatte (✓), Guo Zhang, Gustavo Malkomes (✓), Heta Gandhi (✓), Indra Priyadarsini, James Damewood, James Minuse Stevenson (✓), Jennifer Wei (✓), Juno Nam, Katherine Sytwu (✓), Kevin Jablonka (✓), Kin Long Kelvin Lee (✓), Kiran Vaddi, Kiyou Shibata (✓), L. Catherine Brinson, Luca Thiede (✓), Luis Mantilla (✓), Luis Rangel DaCosta (✓), Manas Likhit Holekevi Chandrappa, Marcel Nassar (✓), Marcelo Finger (✓), Marta Skreta (✓), Marvin Alberts, Mathieu Bauchy (✓), Matteo Aldeghi (✓), Matthew Ryan Hauwiller (✓), Mausam (✓), Mara Schilling-Wilhemi (✓), Martinio Rios-Garcia (✓), Mayk Caldas Ramos (✓), Michał Koziarski (✓), Mikhail Galkin (✓), Milind Malshe, Mingjian Wen, Mingrou Xie, Mohammed Zaki (✓), Moksh Jain (✓), Muratahan Aykol, Nadhir Hassen, Naruki Yoshikawa (✓), Nawaf Alampara (✓), Nofit Segal (✓), Oumar Sekou-Kaba (✓), Pablo Martinez-Crespo (✓), Prashant Govindarajan (✓), Po-An Lin(✓), Rajat Arora (✓), Raj Ghugare (✓), Richard Beckmann (✓), Richard Sheridan (✓), Rob Jordan (✓), Rhys Goodall (✓), Rocío Mercado (✓), Sajid Mannan (✓), Sahil Manchanda (✓), Salome Guilbert, Santiago Miret (✓), Sayan Ranu (✓), Sergio Pablo García Carrillo (✓), Sharath Chandra Raparthy (✓), Shingo Urata (✓), Shujing Wang (✓), Somesh Mohapatra (✓), Sterling G. Baird, Stefano Ribes (✓), Suhas Mahesh (✓), Sulin Liu, Tian Xie (✓), Theo Neukomm, Tong Xie (✓), Tri Minh Nguyen, Sekou-Oumar Kaba (✓), Shuyi Jia, Stefano Martiniani (✓), Vaibhav Bihani (✓), Vahe Gharakhanyan, Victor Schmidt (✓), Vineeth Venugopal (✓), Weike Ye, Xiang Fu, Xiaoxiao Wang (✓), Yao Fehlis (✓), Yao Xuan, Yuan Chiang (✓), Yuta Suzuki, Zhe Liu

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