AI4MAT-ICLR-2025: ICLR 2025 WORKSHOP ON AI FOR ACCELERATED MATERIALS DESIGN

ABSTRACT

AI4Mat-ICLR-2025 explores automating materials discovery via: 1. AI-Guided Design; 2. Automated Chemical Synthesis; 3. Automated Material Characterization inviting discussion on a diversity of leading-edge research at the intersection of machine learning and materials science and engineering.

1 INTRODUCTION

We propose a full-day, medium-sized workshop at ICLR 2025 titled "AI for Accelerated Materials Design" (AI4Mat-ICLR-2025). 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 starting to revolutionize 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 (Radical AI, 2024; CuspAI, 2024; 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.

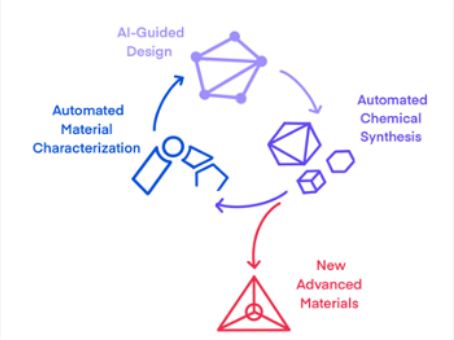

Figure 1: AI-Accelerated Materials Design leveraging 1) AI-Guided Design; 2) Automated Chemical Synthesis; and 3) Automated Material Characterization.

Building on the success of previous AI4Mat workshops at NeurIPS, including AI4Mat-2022, AI4Mat-2023, as well as the upcoming AI4Mat-NeurIPS-2024 workshop, AI4Mat-ICLR-2025 aims to expand the workshop's reach to a broader audience and align with ICLR's focus on multi-modal materials representation. 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 be used to design real-world materials experiments for synthesis and characterization. On top of that, AI4Mat-2023 included 2x the number of accepted submissions, a travel grant program from corporate sponsorships that enabled participation of diverse students, and a themed collection with the prestigious Royal Society of Chemistry *Digital Discovery* journal (Miret et al., 2024). In 2024, AI4Mat-Vienna-2024 and AI4Mat-NeurIPS-2024 continue to build upon the successes of prior workshops, further growing the community and providing a forum for discussion of the most relevant questions at the intersection of AI and materials science. Due to the increased interest from the community, we are proposing AI4Mat-ICLR-2025 to expand AI4Mat to a broader audience while aligning the workshop themes with this rapidly-changing field. With AI4Mat-ICLR-2025 we aim to showcase strong momentum in research activity and provide the opportunity to build and empower an increasingly diverse community seeking to leverage AI for impactful materials applications.

AI4Mat-ICLR-2025 Technical Discussions: The goals of AI4Mat-ICLR-2025 focus on understanding two crucial and unique technical challenges that have emerged in AI for materials design:

1. How Do We Build a Foundation Model for Materials Science? Drawing inspiration from the success of recent foundation models (Bommasani et al., 2021), a plethora of scien-

tific foundation models have been proposed, including some related to materials science (Batatia et al., 2023; Merchant et al., 2023; Takeda et al., 2023; Lee et al., 2023; Yang et al., 2024; Duval et al., 2023). Together, these efforts represent meaningful progress in applying the concept of AI-based foundation models to materials, but individually fall short in addressing a wide range of important materials problems. Given the relevance and growing interest in materials foundation models, we propose a discussion that centers on understanding the complex, interdisciplinary nature of foundational models for materials and how the community can contribute towards building them. To that end, we are bringing together experts from diverse institutions and backgrounds for a forum at AI4Mat-ICLR-2025.

2. What are Next-Generation Representations of Materials Data? As research in AI for materials science has progressed, the materials systems researchers are interested in have become increasingly intricate and diverse as they approach greater relevance for real-world applications. This increase in complexity has renewed questions about how to efficiently represent diverse materials systems (Damewood et al., 2023), including those that might require multiple data modalities. Materials representation learning remains an open problem with unique challenges to be addressed so as to enable continued progress in the development of new machine learning methods for real-world materials challenges.

AI4Mat-ICLR-2025 Community Building: AI4Mat has continued to take intentional steps to provide greater opportunities for this emerging interdisciplinary research community. Our focus remains on providing an inclusive venue for discussion, as well as a space to showcase and amplify high-quality research from an increasingly diverse community. AI4Mat-ICLR-2025 provides a unique opportunity to further grow the community given that it would be the first AI4Mat workshop held in Asia. We aim to take advantage of this opportunity to enable broader participation from previously underrepresented regions, such as South & South-East Asia and the Middle East. Previous AI4Mat workshops had strong representation from North America and Europe, as well as East Asia and South America. To continue to inclusively build the AI4Mat community, facilitate discussion on technical challenges, and encourage networking among participants, we plan to:

1. Travel Grant Program: Building upon the accomplishments of AI4Mat-2023 & AI4Mat-NeurIPS-2024, 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-2025 would provide a unique opportunity to encourage participation from geographically closer regions such as South & South-East Asia and the Middle East through travel grants, who have historically been underrepresented.
2. Tiny Papers Track: Building on the achievements of 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 - Multi-Modal Data for Materials Design: The success of the themed submission track on LLMs for Materials Science at AI4Mat-NeurIPS-2024 prompts us to encourage authors to contribute research along a theme that is aligned with current community-wide research challenges: multi-modal data collection, structured data sharing, and multi-modal representation learning.
4. Journal Track: We also aim to build on the success on AI4Mat-2023's and AI4Mat-NeurIPS-2024 journal track (Miret et al., 2024) to provide AI4Mat researchers the opportunity to submit their work to a prestigious venue for wider recognition.

AI4Mat's Interdisciplinary Research: The interdisciplinary research at AI4Mat-ICLR-2025 represents a growing subfield at the interface of AI and materials science, as evidenced by the greater number of published papers (Butler et al., 2024), new workshops exploring different angles of this emerging intersection (Wang et al., 2023; Regev et al., 2024), as well as large-scale research academic institutes (National Institute of Standards and Technology (NIST), 2024; University of Toronto, 2024; mol, 2023; Pennsylvania State University, 2024; National Science Foundation (NSF), 2024), the continued efforts at large companies (IBM Research, 2024; Merck KGaA and Corporation, 2023; Microsoft Research, 2024; FAIR Chem, 2024) and newly created startups (Radical AI, 2024; CuspAI,

2024; PhaseTree, 2024; Entalpic AI, 2024; Orbital Materials, 2024). Furthermore, AI4Mat intersects with diverse research topics already represented at the ICLR, many of which were accepted to past AI4Mat workshops, including but not limited to: 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.

AI4Mat's Unique Perspective & Distinction from Other ICLR Workshop

Our focus on connecting material scientists and the ICLR community, which has distinct strength in AI techniques, is a unique and valuable approach to sparking discussions related to the interdisciplinary nature of automated materials design. AI4Mat has consistently driven deep technical conversations between materials science and machine learning experts from diverse institutions, drawing speakers, submissions and attendees from both domains. This targeted interdisciplinary approach enables a focus on impactful research problems for materials science that can be effectively tackled with new machine learning methods, making AI4Mat unique from other workshops at ICLR, NeurIPS and ICML. Past ICLR, ICML & NeurIPS workshops in related subject matters have broadly focused on 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 with a heavy emphasis on predictive or generative algorithms. Our proposal differs in that as we aim to shift the focus towards the scientific workflow for the creation of new materials as well as the automation of real-world experiments that can be achieved in each step in this process. Consequently, our proposal takes a holistic approach to automated materials design, and highlights unique research efforts and challenges through our technical program and community-building efforts. Unlike workshops at the broad intersection of AI and the sciences (Maskey et al., 2024; Maddix et al., 2024; Chen et al., 2024), such as ML and the Physical Sciences (Hartman et al., 2024) and AI for Science (Welling et al., 2024), we are targeting a specific focus area that is increasingly important and complementary to the discussions fostered in those workshops.

2 AI4Mat-ICLR-2025 Proposed Workshop

Table 1: Proposed AI4Mat-ICLR-2025 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 - 10.00	Talks + Panel How Do We Build a Foundation Model for Materials Science?	*Workshop Committee & Invited Speakers* **Anima Anandkumar** - Professor, California Institute of Technology **Yousung Jung** - Professor, Seoul National University **Weike Ye** - Research Scientist - Toyota Research Institute Mausam - Professor, Indian Institute of Technology, Delhi
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 What are Next-Generation Representations of Materials Data?	*Workshop Committee & Invited Speakers* **Indra Priyadarsini** - Research Scientist, IBM Tokyo **Xavier Bresson** - Assis. Professor, Nat. Univ. of Singapore **Michael Bronstein** - Professor, University of Oxford **Mustafa Hajij** - Associate Professor, University of San Francisco
15.00 - 15.30	Coffee Break & Networking Tables	*Everyone*
15.30 - 16.15	Spotlights Session	Drawn from Workshop Submissions
16.15 - 17.00	Themed Submission Track Spotlights Session	Drawn from Workshop Submissions
17.00 - 17.15	Closing Remarks & Travel Grant Awards	*Workshop Committee*

Our program focuses on bringing together both AI and materials science experts, with an emphasis on a diverse set of technical perspectives. As such, we have assembled a team of organizers and speakers that span industry and academic institutions across multiple geographies, organizational size, and

levels of seniority. We believe that diverse, multi-institutional perspectives from invited speakers and workshop attendees encourages fruitful technical discussions, as we saw at AI4Mat-2022 & AI4Mat-2023. We regard this as crucial for achieving the goals of AI4Mat-ICLR-2025 to grow both the technical expertise and the research community. Given the increased volume of research relevant to AI4Mat, we expect a medium-sized attendance of $\sim$150 people this year.

2.1 AI4MAT 2022 & AI4MAT-2023 WORKSHOPS

We've based many of our organizational decisions on the successes and shortcomings of the AI4Mat 2022 & AI4Mat-2023 NeurIPS workshops. This includes an emphasis on deep technical discussions of unique challenges in AI for materials design; we focus on timely questions given the rapid progress in the field, as well as continued community-building with greater geographical and demographic representation. AI4Mat22 accepted 40 papers (inc. 12 spotlight) distributed across all three AI4Mat research themes and attracted $\sim$60-70 participants throughout the day. AI4Mat-2023 resulted in 2x the number of submissions with 80 being accepted and 15 spotlights distributed among common submission themes, and attracted $\sim$120 participants. AI4Mat-2022's program focused mainly on lecture-style formats introducing the latest progress in AI-Guided Design, Automated Chemical Synthesis, and Automated Material Characterization at the time. AI4Mat-2023 expanded the program based on the lessons from AI4Mat-2022 and progress in the field, shifting the discussion to real-world materials challenges (Sim2Mat Lightning Talks & Panel) and the emerging role of LLMs for materials (Fireside Chat on LLMs for Materials Design); this was summarized in an openly available perspective presenting the main findings of the workshop discussions and research (Miret et al., 2024). We plan to continue building upon focused, timely discussions that encourage community participation and yield substantive insights in the upcoming AI4Mat-NeurIPS-2024 and in our proposed AI4Mat-ICLR-2025 workshop. AI4Mat-ICLR-2025 provides a unique opportunity to grow the global community of researchers at the forefront of AI and materials science, forging new research collaborations in the community and addressing pressing technical challenges in this emerging subfield.

3 DIVERSITY STATEMENT

We have intentionally selected speakers and committee members with diverse technical viewpoints that will help achieve the complex technical and community-building goals of AI4Mat. For our invited speakers, this includes diversity in: gender (3 women, 5 men); ethnicity; affiliations (6 academia, 2 industry); seniority (industry & government researchers, university faculty, corporate leadership). Our organizing committee members are also diverse in geography, gender, ethnicity, seniority, and other marginalized identities. We plan to phrase our call for submission in an inclusive manner, encouraging submissions and participation from groups with diverse demographic and technical backgrounds across all our tracks, including the Tiny Papers track. We also continue to grow our PC members in a globally inclusive manner, spanning 35 institutions across North & South America, Europe, East Asia, South Asia, and the Middle East for greater geographical representation of researchers engaged in the AI4Mat community. Finally, we will leverage our themed submission tracks for informal mentoring among participants by focusing research discussions on concrete challenges and encouraging the exchange of ideas and formation of new collaborations.

4 LOGISTICS & IMPLEMENTATION

We plan to record or pre-record all presentations, including accepted spotlights and posters, to make the material available online on the workshop website. Our website will provide guidance on when and how to submit contributions, as well as general information on the workshop goals and organizers. We plan to build upon the success of past AI4Mat submission categories (Papers, Tools, Findings, Tiny Papers, and a themed submission track) to encourage a broad set of technical work, especially on the experimental materials side, that can help advance the state-of-the-art and foster discussion among researchers. To assess submitted contributions we will use OpenReview, which includes automatic functionalities for managing conflicts of interest between organizers and reviewers, and require at least 3 reviewers per paper. To reduce potential variance in reviews, we plan to publish the reviewing criteria on the AI4Mat website to make them available to authors and reviewers in advance.

4.1 TIMELINE

- ICLR Decision & Website Update: December 2, 2024 & December 27, 2024
- Submission Deadline & Notification: February 1, 2025 & March 3, 2025
- Workshop: April 27 or April 28, 2025

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

INVITED SPEAKERS

Our invited speakers will share their insights on the major themes of AI4Mat-ICLR-2025 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.

Anima Anandkumar - California Institute of Technology- Google Scholar Website Anima Anandkumar is a well-established research leader in machine learning with extensive academic and corporate experience at NVIDIA and Amazon Web Services. Her experience extends to proposing foundation models for computational biology in proteins as well as recent work more closely aligned to materials science. Anima will bring her diverse technical and non-technical experience to our session How Do We Build a Foundation Model for Materials Science?

Yousung Jung - Seoul National University - Google Scholar Website Yousung Jung is a Professor of Chemical and Biological Engineering at Seoul National University. He has a strong track record of building new machine learning methods to tackle important materials science challenges, such as synthesis and chemical discovery. On top of his academic work, Yousung is involved with multiple industrial and government collaborations in Korea and internationally as a member of the Acceleration Consortium. Yousung's expertise in interdisciplinary machine learning research intersecting with real-world materials challenges will provide a valuable perspective for our session How Do We Build a Foundation Model for Materials Science?

Weike Ye - Toyota Research Institute - Google Scholar Website Weike Ye is researcher at Toyota Research Institute who has focused on developing machine learning methods to address real-world materials design challenges. Her expertise in applying advanced machine learning methods to real-world materials challenges in an industry setting, including recent works on building foundation models, will provide a valuable perspective on the use of foundation models in materials science.

Mausam - Indian Institute of Technology, Delhi - Google Scholar Website Mausam is a Professor of Computer Science at IIT Delhi, and served as the founding head of Yardi School of Artificial Intelligence until September 2023. Mausam's past research has focused extensively on natural language processing with notable recent works on building language models for materials science. The combination of building capable, large-scale models for language along with adapting those techniques towards language models for materials science will provide a valuable perspective in the foundation models session.

Indra Priyadarsini - IBM Tokyo - Google Scholar Website Indra Priyadarsini is researcher at IBM Research, Tokyo, working on accelerated scientific discovery for sustainable materials. Her experience in building machine learning methods for diverse sets of materials for real-world sustainability applications adds to her valuable perspective on next-generation representations for materials data.

Xavier Bresson - National University of Singapore - Google Scholar Website Xavier Bresson is Associate Professor in Computer Science at NUS, Singapore. He is a leading researcher in the field of Graph Deep Learning, including representation learning for diverse fields ranging from scientific applications in quantum chemistry as well as combinatorial optimization and social networks. Xavier's extensive experience in representation learning, including prior work related to materials science, makes him a great fit to speak to Next-Generation Representations of Materials Data, as well as research work on AI for materials science in Singapore.

Michael Bronstein - University of Oxford & AITHYRA Institute- Google Scholar Website Michael Bronstein is a renowned scientist and entrepreneur and research leader in geometric deep learning, currently serving as the DeepMind Professor of Artificial Intelligence in the Computer Science Department at the University of Oxford. Michael's decades-long research leadership in representation learning for complex scientific applications enables him to provide a unique perspective on Next-Generation Representations of Materials Data.

Mustafa Hajij - University of San Francisco Google Scholar Website Mustafa Hajij is an assistant professor in the MSDS program at the University of San Francisco. Mustafa is a research leader in Topological Deep Learning, a newly emerging field with high relevance to representation learning for materials modeling. In addition to his current research work, Mustafa also has research experience in the semiconductor industry as an AI research scientist at KLA Corporation, thereby bringing unique perspectives from both the academic and industrial angles.

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 - Intel Labs (santiago.miret@intel.com) -Google Scholar - LinkedIn Santiago Miret is an AI Research Lead at Intel Labs, where he focuses on research at the intersection of AI and materials science, which builds on his past research experience in AI 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, including the Berkeley Energy & Resources Collaborative (BERC) Energy Summit, which is the largest energy-related conference at UC Berkeley with 1000+ attendees from academia, industry, government, and the general public. Santiago was an organizing committee member for AI4Mat-2022 and AI4Mat-2023, both held at NeurIPS 2022 and NeurIPS 2023 respectively, as well as a committee member of AI4Mat-NeurIPS-2024.

Marta Skreta - University of Toronto (martaskreta@cs.toronto.edu) - Google Scholar - Website Marta is a PhD student in Computer Science at the University of Toronto and Vector Institute working with Alán Aspuru-Guzik under the Canada Graduate Scholarship. Her research focuses on using AI and natural language processing for molecular discovery and decision-making in self-driving labs. Previously, Marta completed internships at Apple and Mila AI for Humanity. She has experience organizing large-scale events, including coding camps for 1000+ Canadian highschool women, and has also been invited as a spotlight speaker at FutureHouse, the Accelerate Conference, and CECAM. Marta was an organizing committee member for AI4Mat-2022 & AI4Mat-2023 and is an active organizer for AI4Mat-NeurIPS-2024.

N. M. Anoop Krishnan - Indian Institute of Technology Delhi (krishnan@iitd.ac.in) - Google Scholar - Website 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), Materials Science and Technology (MST 2019, 2020, 2021, 2022, 2023), 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-2023 at NeurIPS 2023 and is an active organizer for AI4Mat-NeurIPS-2024.

Rocío Mercado Oropeza - Chalmers University (rocio@ailab.bio; rocio.mercado@chalmers.se) - Google Scholar - Website Rocío is an assistant professor in the Computer Science and Engineering

Department at Chalmers University of Technology, where she leads the AI Lab for Molecular Engineering (AIME). She and her team seek to bridge methods from machine learning, chemistry, and the life sciences to engineer molecular systems for therapeutic applications and sustainable materials, focusing on new AI method development. Rocío has significant prior experience in the organization of both online, in-person, and hybrid conferences and workshops, including the annual Broad Institute Machine Learning in Drug Discovery Symposium (MLinDD), Chalmers Structured Learning Workshop, and the Machine Learning for Molecular and Materials Discoveries Symposium (ML2MD). She is also an active organizer of the monthly AI4Science Seminar Series which has hosted >20 early-career international speakers and has >450 subscribers on YouTube. **Rocío is a new organizer for AI4Mat-ICLR-2025.**

Mohamad Moosavi - University of Toronto & Vector Institute & Acceleration Consoritum (mohamad.moosavi@utoronto.ca) - 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 is a new organizer for AI4Mat-ICLR-2025.**

Stefano Martiniani - New York University (sm7683@nyu.edu) - 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 (✓), Amit Gupta (✓), Amol Thakkar, Amuthan A Ramabathiran (✓), Andres Bran (✓), Angel Yanguas-Gil (✓), Anirban Chandra (✓), Anoop Krishnan (✓), Austin Henry Cheng (✓), Ayana Ghosh (✓), Benjamin Manuel Sanchez (✓), Bowen Deng, Carmelo Gonzales (✓), Cheng-Hao Liu (✓), Chenqing Hua (✓), Chenyang Li, Daniel Cassar (✓), Daniel P. Tabor (✓), Daniel Levy (✓), Dorina Weichert, Edward Kim (✓), Elton Pan (✓), Evgeny Burnaev (✓), Emmanuel Bengio (✓), Eric Fuenmueller (✓), Fadwa El Mellouhi, Felix Strieth-Kalthoff (✓), Felix Therrien, Flaviu Cipcigan (✓), Gary Tom (✓), Geemi Wellawatte (✓), George Karypis (✓), Guo Zhang, Gustavo Malkomes (✓), Heta Gandhi (✓), Ilyes Batatia, James Minuse Stevenson (✓), Jennifer Wei (✓), Jennifer D-Souza, Katherine Sytwu (✓), Kevin Jablonka (✓), Kin Long Kelvin Lee (✓), Kiran Vaddi, Kiyou Shibata (✓), 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 (✓), Mayk Caldas Ramos (✓), Michał Koziarski (✓), Mikhail Galkin (✓), Milind Malshe, Mingjian Wen, Mohammed Zaki (✓), Moksh Jain (✓), Muratahan Aykol, Nadhir Hassen, Naruki Yoshikawa (✓), Nawaf Alampara, Nicolas Sawaya (✓), Prashant Govindarajan (✓), Rajat Arora (✓),, Raj Ghugare (✓), Rhys Goodall (✓), Rocio Mercado (✓), Sajid Mannan (✓), Sahil Manchanda (✓), Santiago Miret (✓), Sayan Ranu (✓), Sergio Pablo García Carrillo (✓), Simon Batzner, Sharath

Chandra Raparthy (✓), Shingo Urata (✓), Somesh Mohapatra (✓), Sterling G. Baird, Suhas Mahesh (✓), Sulin Liu, Tian Xie (✓), Tong Xie (✓), Tri Minh Nguyen, Sekou-Oumar Kaba (✓), Stefano Martiniani (✓), Vaibhav Bihani (✓), Vahe Gharakhanyan, Victor Schmidt (✓), Vineeth Venugopal (✓), Xiaoxiao Wang (✓), Yao Fehlis (✓), Yao Xuan, Yuta Suzuki, Zhe Liu

REFERENCES

Molecule maker lab institute, 2023. URL https://moleculemaker.org/.

I. Batatia, P. Benner, Y. Chiang, A. M. Elena, D. P. Kovács, J. Riebesell, X. R. Advincula, M. Asta, W. J. Baldwin, N. Bernstein, et al. A foundation model for atomistic materials chemistry. *arXiv preprint arXiv:2401.00096*, 2023.

R. Bommasani, D. A. Hudson, E. Adeli, R. Altman, S. Arora, S. von Arx, M. S. Bernstein, J. Bohg, A. Bosselut, E. Brunskill, et al. On the opportunities and risks of foundation models. *arXiv preprint arXiv:2108.07258*, 2021.

K. T. Butler, K. Choudhary, G. Csanyi, A. M. Ganose, S. V. Kalinin, and D. Morgan. Setting standards for data driven materials science. *npj Computational Materials*, 10(1):231, 2024.

W. Chen, P. Ren, E. Massara, Y. Wang, B. Erichson, L. Perreault-Levasseur, B. Li, and S. Chaudhuri. Foundation models for science: Progress, opportunities, and challenges - neurips 2024, 2024. URL https://fm-science.github.io/index.html.

CuspAI. Cuspai secures 30m to combat climate change with ai-designed materials, 2024. URL https://www.cusp.ai/.

J. Damewood, J. Karaguesian, J. R. Lunger, A. R. Tan, M. Xie, J. Peng, and R. Gómez-Bombarelli. Representations of materials for machine learning. *Annual Review of Materials Research*, 53(1): 399–426, 2023.

A. Duval, S. V. Mathis, C. K. Joshi, V. Schmidt, S. Miret, F. D. Malliaros, T. Cohen, P. Liò, Y. Bengio, and M. Bronstein. A hitchhiker's guide to geometric gnns for 3d atomic systems. *arXiv preprint arXiv:2312.07511*, 2023.

Entalpic AI. Entalpic ai, 2024. URL https://entalpic.notion.site/Entalpic-is-hiring-9f29b9a69fb840508cd3f9a7c1c0d057.

FAIR Chem. Fair chemistry, 2024. URL https://fair-chem.github.io/. Accessed: 2024-10-02.

N. Hartman, V. Mikuni, S. Mishra-Sharma, M. Pettee, S. Wagner-Carena, and A. Wehenkel. Machine learning and the physical sciences - neurips 2024, 2024. URL https://ml4physicalsciences.github.io/2024/.

IBM Research. Ai for scientific discovery, 2024. URL https://research.ibm.com/projects/ai-for-scientific-discovery.

K. L. K. Lee, C. Gonzales, M. Spellings, M. Galkin, S. Miret, and N. Kumar. Towards foundation models for materials science: The open matsci ml toolkit. In *Proceedings of the SC'23 Workshops of The International Conference on High Performance Computing, Network, Storage, and Analysis*, pages 51–59, 2023.

C.-H. Liu, J. Rector-Brooks, J. Yim, S. Yang, S. Lisanza, F.-Z. Li, P. Chatterjee, T. Jaakkola, R. Barzilay, D. Baker, F. H. Arnold, and Y. Bengio. Integrating generative and experimental platforms or biomolecular design. In *ICLR 2024 Workshops*, 2024. URL https://openreview.net/forum?id=FyX6sshjgg.

D. C. Maddix, S. Alizadeh, B. Han, A. S. Krishnapriyan, N. Ashton, V. Benson, M. Reichstein, B. Wang, M. Zarekarizi, M. W. Mahoney, A. G. Wilson, and G. Karypis. AI4differentialequations in science. In *ICLR 2024 Workshops*, 2024. URL https://openreview.net/forum?id=LQVSPCgHqF.

M. Maskey, L. Bat-Leah, D. Brajovic, P. Climaco, A. Parrish, C. Park, X. Yao, H. Caesar, B. Koch, F. Alzamzami, Z. Wang, J. Andrews, P. Paritosh, S. Vogler, M. F. Chen, S. T. Truong, and B. Ma. Data-centric machine learning research (DMLR): Harnessing momentum for science. In *ICLR 2024 Workshops*, 2024. URL https://openreview.net/forum?id=5y6fLlZhcO.

A. Merchant, S. Batzner, S. S. Schoenholz, M. Aykol, G. Cheon, and E. D. Cubuk. Scaling deep learning for materials discovery. *Nature*, 624(7990):80–85, 2023.

G. Merck KGaA, Darmstadt and I. Corporation. Merck kgaa, darmstadt, germany and intel accelerate sustainable semiconductor processes and manufacturing technologies through academic research in europe, 2023. URL https://www.emdgroup.com/en/news/semiconductor-manufacturing-09-03-2023.html.

Microsoft Research. Microsoft research ai4science lab, 2024. URL https://www.microsoft.com/en-us/research/lab/microsoft-research-ai4science/. Accessed: 2024-10-02.

S. Miret, M. Skreta, B. Sanchez-Lengelin, S. P. Ong, Z. Morgan-Chan, and A. Aspuru-Guzik. Ai4mat: Ai for accelerated materials design neurips 2022 workshop, 2022. URL https://sites.google.com/view/ai4mat.

S. Miret, N. A. Krishnan, B. Sanchez-Lengeling, M. Skreta, V. Venugopal, and J. N. Wei. Perspective on ai for accelerated materials design at the ai4mat-2023 workshop at neurips 2023. *Digital Discovery*, 2024.

N. NaderiAlizadeh, S. Sledzieski, K. Jha, M. Kshirsagar, R. Singh, and Q. Justman. Accessible and efficient foundation models for biological discovery - icml 2024, 2024. URL https://accml.bio/.

National Institute of Standards and Technology (NIST). CHIPS R&D Funding Opportunities, 2024. URL https://www.nist.gov/chips/chips-rd-funding-opportunities.

National Science Foundation (NSF). National artificial intelligence research institutes (nsf 23-610) solicitation, 2024. URL https://new.nsf.gov/funding/opportunities/national-artificial-intelligence-research-institutes/nsf23-610/solicitation.

Orbital Materials. Orbital materials, 2024. URL https://www.orbitalmaterials.com/.

Pennsylvania State University. Institute for ai-enabled materials discovery, design, and synthesis, 2024. URL https://www.icds.psu.edu/institute-for-ai-enabled-materials-discovery-design-and-synthesis/.

PhaseTree. Phasetree, 2024. URL https://www.phasetree.ai/.

Radical AI. About radical ai, 2024. URL https://www.radical-ai.com/about.

A. Regev, A. Volkamer, B. Trentini, C. Clementi, C. Harris, C. Deane, C. Dallago, E. Zhong, F. Grisoni, J. Leem, K. Yang, M. Segler, M. Pieler, N. Sofroniew, O. Viessmann, P. Koo, P. Chatterjee, P. V. Gerwen, R. Lindsay, U. Lupo, and Y. W. Li. Ml for life and material science: From theory to industry applications, 2024. URL https://ml4lms.bio/.

S. Takeda, A. Kishimoto, L. Hamada, D. Nakano, and J. R. Smith. Foundation model for material science. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 37, pages 15376–15383, 2023.

M. Uehara, M. Wang, S.-I. Lee, L. Song, N. Richmond, M. Brbic, M. Lotfollahi, , X. Li, and E. Hajiramezanali. Ai for new drug modalities - neurips 2024, 2024. URL https://sites.google.com/view/newmodality-aidrug.

University of Toronto. U of t receives $200-million grant to support acceleration consortium's self-driving labs research, 2024. URL https://www.utoronto.ca/news/u-t-receives-200-million-grant-support-acceleration-consortium-/s-self-driving-labs-research.

H. Wang, S. Batzner, T. Xie, and X. Fu. Ml4materials from molecules to materials, 2023. URL https://www.ml4materials.com/.

M. Welling, M. Zitnik, C. P. Gomes, T. Jaakkola, P. Dayan, Y. Du, A. Fang, L. Cheng, K. W. Li, B. Jing, and D. Luo. Ai for science: Scaling in ai for scientific discovery - icml 2024, 2024. URL https://ai4sciencecommunity.github.io/icml24.html.

H. Yang, C. Hu, Y. Zhou, X. Liu, Y. Shi, J. Li, G. Li, Z. Chen, S. Chen, C. Zeni, et al. Mattersim: A deep learning atomistic model across elements, temperatures and pressures. *arXiv preprint arXiv:2405.04967*, 2024.