AI for Materials Design Workshop explores needed research directions

By **Vineeth Venugopal**

The second AI for Accelerated Materials Design (AI4Mat) Workshop took place on December 15, 2023, as a segment of the 37th Annual Conference on Neural Information Processing Systems (NeurIPS), hosted in New Orleans, La., from December 10 to 16, 2023. AI4Mat focused on the integration of artificial intelligence (AI) and materials science, led by an organizing committee from both academia and industry, with objectives to present recent progress, stimulate discussions, and explore collaborative research directions.

In its second year, AI4Mat-2023 featured a collection of 85 posters from international researchers, alongside 25 carefully selected spotlighted talks drawn from the paper submissions. The event included keynote presentations that delved into the relationship between AI and materials science, highlighting the latest research and applications in this dynamic field.

Kicking off the workshop's invited sessions, experts from leading research institutions and industry shared insights on the synergy between AI and materials science. Rama K. Vasudevan at Oak Ridge National Laboratory, Maria Chan from Argonne National Laboratory, and Vijay Narasimhan from EMD Electronics spoke at the first invited session in the morning. Vasudevan highlighted the necessity of human intuition in autonomous experiment platforms for microscopy and spectroscopy, indicating that while fully autonomous systems are challenging, human curiosity can guide AI. Chan discussed the importance of understanding structures at the nanoscale and developing universal models to translate structural data into materials properties, showcasing the machine learning/AI framework FANTASTX to expedite this process. Narasimhan underscored the role of digital tools in accelerating industry development, pointing to the environmental impact of materials like PFAS and the potential of generative AI and large data sets for innovation in the semiconductor industry.

In the panel discussion that followed, the speakers emphasized the potential of data sets, to further research at the intersection of AI and materials science particularly in metal organics and thin-film synthesis. Federated data sets, where multiple parties contribute jointly for greater data sharing, improving the quality and benchmarking of density functional theory data sets, and integrating more metadata were highlighted as crucial steps. The discussion also touched on making infrastructure robust, addressing the digital gap in semiconductors, and the importance of community tools like user facilities and public domain software for sustainability. The future role of AI as an extension of scientists, enabling a focus on core scientific inquiries, and the challenges in materials science at various scales were discussed, underscoring the already real impact of AI4Mat and the anticipation of its broader application as experimental and simulation workflows mature.

The afternoon's highlight was a fireside chat on Large Language Models (LLMs) in Materials Design, with Andrew White from the University of Rochester, Gowoon Cheon from Google DeepMind, and Gabriel dos Passos Gomes from Carnegie Mellon University. They explored LLMs' potential in materials synthesis over prediction, emphasizing the importance of human intuition alongside the challenges of data set integrity, standardization, and improving LLM reliability. The discussion spanned tool augmentation, reasoning evaluation, structured knowledge integration, and LLMs' promising applications in organic chemistry and materials science, highlighting their transformative yet cautiously observed impact on scientific exploration and future applications.

The AI for Materials Science (AI4Mat) Workshop was held on December 15, 2023, as part of NeurIPS in New Orleans, La. Pictured here are recipients of travel awards, along with the workshop organizers.

A notable outcome was the consensus on the need for a collaborative approach that integrates human intuition with AI technologies. The workshop highlighted several pioneering frameworks and methodologies for accelerating data to application processes, and the application of machine learning in generating synthetic data for new materials development. The discussions underscored the importance of creating impactful data sets and improving infrastructure to support AI4Mat research.

By bringing together leading experts and emerging researchers, the AI4Mat workshop facilitated a rich exchange of ideas and set the stage for groundbreaking advancements in the integration of AI with materials science. This year, for the first time, 10 travel awards were dispersed to participants from underrepresented communities, students, and other deserving individuals due to a generous contribution from Intel Labs. The workshop was organized by N M Anoop Krishnan from the Indian Institute of Technology Delhi; Santiago Miret from Intel Labs; Benjamin Sanchez-Lengeling from Google DeepMind, Marta Skreta from the University of Toronto; Vineeth Venugopal from the Massachusetts Institute of Technology; and Jennifer N. Wei from OpenFold, Open Molecular Software Foundation. □