



Scientific generative AI and materials science: From prediction to physical intelligence

By Blessing Ishola and Corrisa Heyes

In March 2025, the Materials Research Society (MRS), in collaboration with *Nature*, hosted a two-day virtual workshop focused on the transformative role of artificial intelligence (AI) in materials science. Workshop organizers **Markus Buehler**, from the Massachusetts Institute of Technology (MIT) and *Impact* editor of *MRS Bulletin*, and **Kristina Karch**, senior editor for materials science for *Nature*, brought together researchers from academia, industry, and publishing to explore the integration of machine learning (ML), generative models, quantum computing, and automation across the research pipeline. Rather than isolating tools and techniques, the workshop emphasized a systems-level approach where AI reshapes how materials are simulated, discovered, and designed. Three themes emerged: accelerating multiscale modeling, integrating AI across scientific infrastructure, and advancing generative and embodied intelligence.

Accelerating multiscale modeling through machine learning

A major focal point was the growing use of ML surrogates and coarse-grained models to accelerate simulation workflows. **Michele Ceriotti** (École Polytechnique Fédérale de Lausanne) introduced surrogate models powered by equivariant neural networks to replicate electronic structure calculations. His research team's hybrid strategy, blending fast predictions with periodic quantum mechanical corrections, reduces computational costs without sacrificing physical accuracy. These techniques broaden accessibility, enabling reliable simulations even outside the realm of computational specialists. Expanding on this approach, **Cecilia Clementi** (Freie Universität Berlin) demonstrated how coarse-grained techniques like CGSchNet and variational force matching can capture long-time scale behavior in molecular systems. These models

facilitate high-throughput exploration of chemical variability, although challenges persist in modeling long-range interactions.

Max Welling (University of Amsterdam) contextualized these developments as part of a shift from data-driven modeling to full *in silico* emulation. His BARNN model incorporates Bayesian learning and uncertainty quantification to support trustworthy predictions. Meanwhile, **Xiaoying Zhuang** (Leibniz Universität Hannover) showcased how models trained on density functional theory data can propagate predictions up to the continuum scale, capturing properties like fracture toughness and elasticity. Her multiscale framework supports both predictive and inverse design goals, integrating physics-informed ML with practical performance metrics. Rounding out the theme, **Simon Batzner** (Google DeepMind) emphasized that model performance must align with synthetic feasibility.

His group's GNoME platform incorporates decomposition enthalpy as a stability metric to bridge the gap between theoretical discovery and real-world fabrication.

Integrating AI across the scientific infrastructure

Chi Chen (Microsoft Azure Quantum) explored the infrastructural dimension of AI in materials research where AI, high-performance computing, and quantum computing converge. While quantum platforms are not broadly faster than classical systems, they

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are well suited to optimization tasks in chemistry. Chen emphasized the importance of user-friendly infrastructure to support broad adoption of these tools.

In a panel discussion, speakers addressed questions ranging from quantum computing applications to the future of scientific labor. They emphasized that while AI models are growing more complex and powerful, their usability and trustworthiness remain a potential stumbling block. Several panelists noted that scientists should be directly involved in tool development to preserve creativity and professional judgment. Discussions also touched on the importance of foundational training in programming, mathematics, and statistics. These skills enable researchers to critically evaluate AI-generated results, especially when predictions fall outside expected bounds. Despite concerns about shifting roles, the consensus was clear: scientists remain essential to guide, interpret, and challenge AI systems.

Generative and embodied intelligence for design

The last day of the workshop shifted to the creative and generative potential of AI. Rather than merely predicting materials properties, researchers are using AI to propose new materials, structures, and mechanisms tailored to user-defined goals. **Cate Brinson**

(Duke University) shared her research team's work with large language models (LLMs) for scientific knowledge extraction. By converting unstructured data like figures and tables into structured data sets, they are developing benchmarks to evaluate LLMs in scientific contexts. These tools aid in data curation and model interpretation, pushing LLMs toward more rigorous scientific utility.

Extending his earlier focus on uncertainty, Welling described how surrogate models not only emulate behavior but also drive design by optimizing confidence-weighted outcomes. His examples included climate models and chemical design, and he highlighted the launch of his startup CuspAI for industrial and environmental applications.

Building on the generative theme, **Johnson Tsun-Hsuan Wang** (MIT) described systems that co-optimize morphology and motion. His diffusion-based models respond to human input and simulation feedback, guiding robot designs from abstract objectives to physical instantiation. Wang noted current fabrication challenges but emphasized that embodied intelligence will be crucial to next-generation AI applications. At the molecular level, **Rose Cersonsky** (University of Wisconsin–Madison) focused on model intentionality, ensuring that ML systems are trained to retain chemically

meaningful features. Her research group's use of custom loss functions and careful descriptor mapping helps preserve interpretability and domain relevance. Zhuang's multiscale framework, revisited here, complements these approaches by enabling inverse design workflows that start with target properties and back-calculate structural configurations, enhancing the feasibility and utility of AI-generated materials.

Conclusion: Toward a convergent AI framework

Throughout the event, it became clear that AI in materials science is evolving from a computational shortcut into a central design philosophy. From simulation to generative design, and from scientific practice to physical systems, AI is not replacing researchers; it is extending their reach by capitalizing on quick and effective runs for informative reasoning and learning before an experimental procedure. Its power depends on engagement: on researchers' understanding how models operate, what data they learn from, and what design logic they encode. When deployed thoughtfully, AI can help unify modeling, synthesis, and experimentation into a cohesive, adaptive, and creative scientific workflow.

This workshop made a compelling case for the future of AI and the role of scientists in shaping it. ☐



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