Trustworthy Multi-Model AI for Materials Discovery: From Scientific Knowledge to Auditable Industrial Decision-Making

Speaker

Amine Mohamed
Founder & President, Korev AI
Grenoble, France

Abstract

Artificial intelligence is opening new possibilities for materials discovery by enabling researchers to navigate large scientific corpora, combine heterogeneous sources of knowledge and data, and explore candidate hypotheses at a scale that would be difficult to achieve through human analysis alone.

As these capabilities move closer to experimental and industrial workflows, however, a critical question emerges: how can an AI-generated hypothesis be sufficiently qualified and trusted before computational, experimental or industrial resources are committed to testing it?

This contribution explores a trustworthy multi-model approach designed to support the transition from scientific knowledge to auditable decision-making in materials discovery.

The proposed architecture combines heterogeneous AI models with scientific literature, materials data and domain-specific knowledge. Rather than relying on the output of a single model, several models can independently analyse a scientific question, formulate or evaluate hypotheses, identify supporting evidence and expose uncertainty or disagreement.

The objective is not simply to produce a majority answer. Agreement between models can strengthen a hypothesis, while disagreement can itself become valuable information by revealing uncertainty, conflicting evidence or areas requiring further scientific investigation.

The resulting hypotheses can then be consolidated while preserving the provenance of the underlying sources, the contributions of the different models, identified uncertainties and the successive steps that led to their qualification. This creates a traceable pathway between scientific information, AI-assisted exploration and the decision to proceed toward simulation, laboratory experimentation or industrial evaluation.

Human expertise remains central to this architecture, but not merely as a final validation layer added to an autonomous system. The underlying principle is one of complementary intelligence.

AI can mobilise and compare large volumes of scientific knowledge, detect relationships across heterogeneous information and explore a broader hypothesis space. Scientists and domain experts contribute different and indispensable capabilities: contextual understanding, tacit knowledge, experimental intuition, scientific judgment and responsibility.

The objective is therefore not to make humans and machines perform the same cognitive task, nor to remove the scientist from the decision process, but to organise their collaboration according to their respective strengths. Human experts retain the ability to challenge, refine, reject or approve AI-generated hypotheses before they progress toward experimentation or industrial decision-making.

Applied to materials discovery, such an approach could help researchers and industrial teams prioritise which hypotheses deserve further investigation while maintaining traceability over why they were selected.

Ultimately, the challenge is not only to use AI to generate more hypotheses or explore materials faster. It is to establish a trustworthy path from what AI makes possible to explore to what scientists decide is meaningful enough to test.