

AI-driven Materials Science

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ABSTRACT

Artificial intelligence is rapidly reshaping materials science, offering new possibilities for accelerating simulations, guiding experiments, and even generating scientific hypotheses. Yet the path toward truly autonomous discovery remains limited by three long-standing challenges: quantum-level simulations remain expensive, experimental validation is slow and resource-intensive, and language models often inherit biases from the scientific literature. In this seminar, I will discuss how emerging AI techniques can confront these issues through accelerated computational models, autonomous experimental platforms, and materials-aware language models capable of scientific reasoning. By integrating these elements into a closed-loop system, AI can move from passively predicting properties to actively exploring and testing scientific ideas. The seminar will outline the emerging landscape of such autonomous materials discovery systems and discuss how they can reshape future scientific research.