

Materials discovery: the role of Networks and AI

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The discovery and optimization of novel material finds application across diverse technologies, from energy storage and catalysis to electronics and structural applications. Yet, the immense size of chemical space and the intricate links between composition, structure, and properties render traditional trial-and-error methods slow and inefficient. Recent developments in artificial intelligence (AI) and network science offer powerful avenues to accelerate this process, enabling rapid prediction, design, and optimization of materials with tailored properties. This review examines how machine learning (ML) and network theory are reshaping the landscape of materials discovery.

