Inverse Materials Design

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The inverse materials design problem (given a target property or function, identify the optimal material) represents one of the central challenges in materials science. The landscape of materials theory and simulation is adapting to solve this problem with the integration of new techniques and tools from the artificial intelligence community. Progress in hardware, including classical supercomputers and emerging quantum computers, alongside software advancements incorporating advanced algorithms and statistical machine learning models, is expanding what is now possible [1]. Developments such as large language models and generative diffusion techniques are unlocking application areas ranging from multimodal characterisation to direct integration with self-driving laboratories. I will survey the evolution of data-driven approaches to inverse materials design, highlighting their potential to expedite the identification of compounds essential for the next generation of clean energy technologies [2]. Recent progress for crystalline materials will be covered, while addressing persistent obstacles such as reliable structure-property databases that underpin models which are repeatable, reproducible, and robust [3].

References

[1] *"Machine learning for molecular and materials science"* K. T. Butler et al, Nature, 559 (2018) 547.
[2] *"Exploration of crystal chemical space using text-guided generative artificial intelligence"* H. Park, A. Onwuli, A. Walsh, Nature Communications 16 (2025) 4379.
[3] *"Open computational materials science"* A. Walsh, Nature Materials 23 (2024) 16.