Exploring New Frontiers in Inverse Materials Design through Graph Neural Networks and Large Language Models

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Finding new materials with suitable properties has been a challenging task due to computational and experimental costs. Inverse design approaches enable the establishment of a property-to-structure model, rather than the traditional structure-to-property model development. Such approaches can surpass traditional funnel-like materials screening methods and facilitate the computational discovery of next-generation materials. In this talk, we will explore the application of graph neural networks and the recently popular large language models to the forward and inverse design of materials, specifically semiconductors and superconductors. We will compare and understand the strengths and limitations of these approaches. The materials predicted by inverse models are further validated using density functional theory before experimental synthesis and characterization.

References

[1] K. Choudhary, AtomGPT: Atomistic Generative Pre-trained Transformer for Forward and Inverse Materials Design, arXiv:2405.03680 (2024)

[2] D. Wines, T. Xie, K. Choudhary, Inverse design of next-generation superconductors using data-driven deep generative models, J. Phys. Chem. Lett., 14, 6630 (2023)

[3] K. Choudhary et al., JARVIS-Leaderboard: a large scale benchmark of materials design methods, npj Computational Materials 10, 93 (2024)

Figures

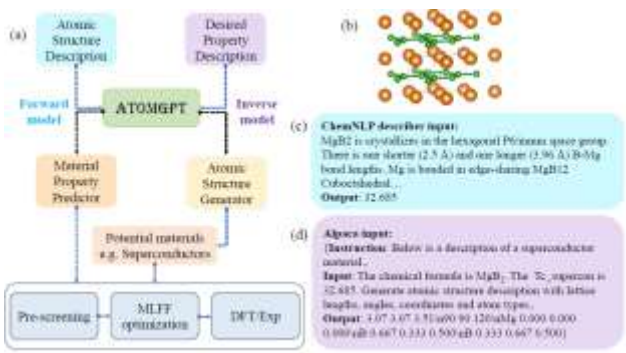

Figure 1. Schematic overview of forward and inverse materials design.