Exploring the Impact of Generative AI Algorithms for Advanced Battery Material Analysis

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ABSTRACT

The emergence of Generative Artificial Intelligence (GAI) presents a paradigm shift in materials research [1], promising high insights into structure-activity relationships. However, this revolution faces difficulties due to inadequate progress in data quality governance and the absence of guidelines on integrating domain knowledge with data-driven analysis.

Several pivotal challenges should be addressed to generalize the use of GAI in material science: balancing the high dimensionality of feature space against low variability and small size of sample datasets, reconciling prediction accuracy with interpretability and mitigating artefacts and hallucinations in generated data.

GAI pave the way of new possibility on correlative study based on multimodal analysis. Moreover, integrating pre-trained LLM models with multimodal and multivariate GAI models unlocks novel capabilities, facilitating the construction of multimodal LLM frameworks [2]. These frameworks offer enhanced insights into material properties and uncover hidden correlated behaviors, incorporating prompt paradigm and reinforcement learning from human feedback.

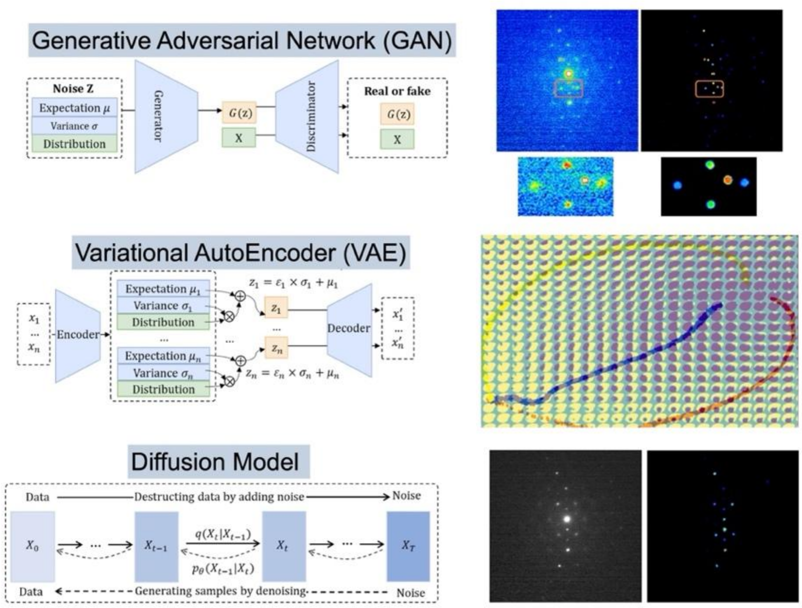

Figure 1. **Generative AI models.** (a) Generative adversarial Network (GAN) for electron diffraction pattern denoising, (b) Variational AutoEncoder (VAE) for accelerating phase field simulation, (c) Diffusion Model for denoising of 4D-STEM patterns and TEM images [1].

On the other hand, physics-based models such as phase field simulations, which delve into lithiation dynamics within single cathode crystals, are computationally intensive and time-consuming. To tackle this challenge, Variational Auto-Encoders (VAEs) present a data-driven approach, accelerating drastically the simulation process [3,4]. Additionally, emerging physics-informed algorithms offer a novel strategy [5], utilizing experimental datasets and constrained models with integrated physics equations in loss functions to simulate complex systems. GANs (including Pix2Pix GAN and CycleGAN) [6] and Diffusion algorithms [7] are actively developed for dataset denoising prior to processing. Evaluation of the efficiency and limitations, including artifact presence, of these algorithms in denoising 4D-STEM diffraction patterns and TEM images has been conducted [8,9].

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