Data driven design and analysis of advanced battery materials

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The development of advanced battery materials has traditionally relied on physics-based simulations and experimental characterization to evaluate structure–property relationships and performance. While effective, these approaches often involve long development cycles that limit rapid exploration of large and high-dimensional design spaces. Data-driven methods offer a complementary pathway by enabling efficient knowledge extraction across diverse simulation and experimental datasets. In particular, deep learning techniques offer powerful tools for modeling, interpreting, and navigating high-dimensional data. In this talk, I will present a coupled generative–discriminative deep learning framework designed to accelerate the early-stage screening, characterization, and guided discovery of battery material systems. Generative models learn underlying data distributions and enable exploration of candidate designs, while discriminative models extract compact, informative latent representations that capture salient structural and functional features. Integrating these complementary learning paradigms supports both expansion and distillation of knowledge within complex design spaces. I will illustrate the framework across several application modes, including learning latent representations of system formation and evolution from simulation-derived descriptors, automatically discovering structure and composition from characterization data, and early-stage screening of candidate materials based on functional properties before downstream validation.

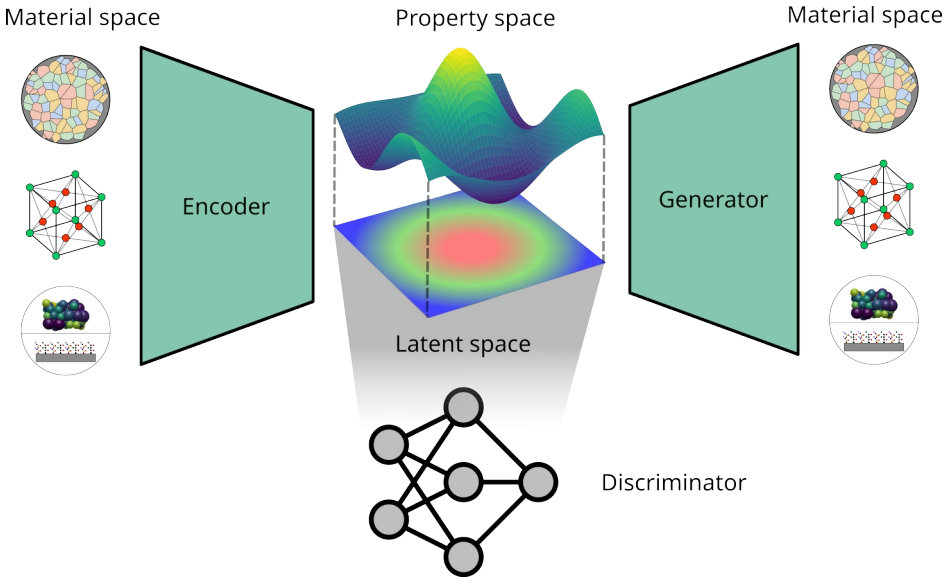

Figure 1. Overview of the generative–discriminative framework showing contraction of high-dimensional material data into informative latent representations and expansion from latent space to data space.