Generative Models for Crystalline Materials Design

Kinga O. Mastej[1], Aron Walsh[2]
[1]Imperial College London, Address, Exhibition Rd, London SW7 2AZ, UK
[2]Imperial College London, Address, Exhibition Rd, London SW7 2AZ, UK

k.mastej24@imperial.ac.uk

Crystalline materials are vital to clean energy technologies, enabling applications such as solar energy conversion and electrochemical energy storage. This research explores the use of generative artificial intelligence (AI) models for accelerated design of crystalline materials with enhanced performance and sustainability. Central to this approach is the development of advanced representations that encode materials into an informative latent space, preserving key physicochemical properties and crystallographic symmetries. Generative models, including variational autoencoders, transformers, and reinforcement learning frameworks, are employed to navigate this latent space, enabling the prediction and virtual screening of novel materials with tailored properties prior to experimental synthesis. This iterative design loop promises to expand the search for promising materials across a vast combinatorial design space. The project's outcomes target critical performance metrics related to electronic, ionic, and thermal properties in crystals, with potential applications in next-generation energy technologies. By integrating computational chemistry, machine learning, and materials science, this research aims to advance the discovery of high-performance, sustainable materials for energy systems