### Machine learning-enabled acceleration of catalyst developments

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The traditional Edisonian approach to material development is notoriously slow and costly, often requiring over 20 years and billions of dollars to bring a single material from discovery to commercialization. In contrast, data science and machine learning (ML) have the potential to exponentially accelerate this process, which has attracted significant attention in materials science for the last decade.

This talk will be divided into two chapters, both of which demonstrating ML-enabled accelerations of catalyst developments. In the first chapter, I will explore how graph neural networks can accelerate the discovery of novel catalysts, with a particular focus on fuel cell catalysts as a case study. Additionally, I will present ML-enabled investigations into the stability of real-scale nanoparticles in electrochemical environments, a challenge previously unattainable through conventional methods. The second chapter will focus on autonomous material synthesis based on ML optimization methods, such as Bayesian active learning. I will demonstrate the development of water splitting catalysts designed to simultaneously meet both activity and stability criteria using this approach.