Accelerated Catalyst Discovery from First Principles Simulations and Machine Learning

백서인†
서강대학교 화공생명공학과
(sback@sogang.ac.kr†)

Towards a sustainable energy future, it is essential to develop new catalysts with improved properties for key catalytic systems such as water electrolysis and fuel cell. Unfortunately, the current state-of-the-art catalysts still suffer from the high cost of noble metals, insufficient catalytic activity, and long-term stability. Atomic simulations have demonstrated the potential to design new catalysts to overcome the current challenges. For the past decades, atomic simulations have become reasonably accurate and high-throughput calculations for catalyst screening have become feasible due to the exponential increase in computing power. More excitingly, recent advances in machine learning have opened up the possibility to reduce the number of density functional theory (DFT) calculations for high-throughput catalyst screening.

In this talk, I will demonstrate recent atomic simulation results on developing new catalysts for oxygen electrochemistry and discuss how machine learning could be of help to accelerate catalyst discovery. The current challenges in the computational catalysis field toward an accurate and efficient catalyst discovery will also be discussed.