원자 레벨 시뮬레이션을 통한 합리적인 전기화학 촉매 설계

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The development of active, stable and cost-effective alternative catalysts has been of utmost focus in renewable and sustainable future energy technologies such as hydrogen peroxide production, ammonia production, fuel cells and electrolyzers. Unfortunately, the current brute-force approach is nearly impossible to investigate all possible combinations from the broad chemical space. To overcome the current scientific challenges, atomic simulations have demonstrated the potential to accelerate the discovery of new catalysts. More excitingly, recent advances in machine-learning have opened up the possibility of high-throughput catalyst screening with the minimal number of expensive density functional theory (DFT) calculations. In this talk, I will discuss how atomic simulations and machine learning-assisted high-throughput screening can accelerate the discovery of new catalysts for various electrochemical reactions. Not only the catalytic activities, but many other important factors have been considered to bridge the gap between simulations and experiments.