# Understanding Reaction Mechanisms and Catalytic Activities of Electrochemical Ammonia Oxidation on Transition Metals

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To produce green $H_2$, oxygen evolution reaction (OER) has been intensively investigated in the past decade, although a large overpotential and harsh operating potential have been considered as bottlenecks for a commercialization. As an alternative, $NH_3$ oxidation has gained attention recently.

$NH_3$ electrooxidation reaction has a great potential for $H_2$ production, because it theoretically requires 98 % less energy than OER considering the equilibrium potentials (0.03 $V_{RHE}$ for $H_2/NH_3$ vs. 1.23 $V_{RHE}$ for $H_2/H_2O$). Among pure metals, Pt is known to exhibit the best catalytic activity, where overpotential is around 0.50 V. To discover new catalysts that outperform Pt, fundamental studies on activities and reaction mechanisms are required.

In this talk, I'll discuss systematic computational results for $NH_3$ electrooxidation on 26 transition metals. We considered all possible reaction pathways, thermo-coupling, electrochemical and combined ones, resulting in total 9 pathways. By performing a microkinetic analysis, we determined the most favorable pathway for each catalyst, and we propose a catalyst design strategy by finding activity descriptors and constructing kinetic volcano plot.