Discovery of Single Atom Catalysts Supported by Two-dimensional Materials for Electrochemical Ammonia Oxidation

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One of the current state-of-the-art technologies to produce green H_2 gas is through H_2O electrolysis, where H_2O is oxidized to O_2 at the anode (E°=1.23 V_{RHE}) and H_2 is produced at the cathode (E°=0.00 V_{RHE}) with the thermodynamic potential of 1.23 V. Alternatively, ammonia (NH_3) oxidation (E°=0.07 V_{RHE}) can take place at the anode, reducing the thermodynamic potential by 94 % compared to the H_2O electrolysis. Pt catalysts demonstrated decent catalytic activities for NH_3 oxidation with the observed overpotential of 0.6 V, and 0.3 V when alloyed with Ir and Ru. However, no literature focusing on single atom catalysts for NH_3 oxidation has been reported to date. In this talk, I will discuss density functional theory (DFT) calculation results on graphene-supported single metal atom catalysts to understand the reaction pathway and catalytic activity for NH_3 oxidation. Based on the calculated results, we develop a machine learning model to efficiently predict the catalytic properties of new materials, which is then used to screen ~800 new single atom catalysts. Considering the activity and stability, we suggest new catalysts which could outperform the state-of-the-art Pt catalyst.