

# Rational design of metalloporphyrin oxygen reduction catalysts

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The development of hydrogen fuel cell technologies is a key piece of the renewable energy puzzle, but these technologies have yet to reach their full potential. These devices generate electricity from the conversion of oxygen gas and hydrogen gas into water. In contemporary devices, this interconversion is optimized through the use of platinum catalysts, but their high cost and low abundance in nature makes the widespread adoption of fuel cell technologies in their current state unlikely. Thus, the development of effective, low-cost, and earth abundant cathode catalysts would greatly increase the potential of these technologies. The vast size of the chemical space makes direction from computational modeling especially necessary in the development of new catalysts. One class of molecules that has particular promise for oxygen reduction catalysis is the metalloporphyrins. The planar geometry of these compounds makes them ideal for the binding of catalytic substrates as well as allowing for systematic modification of the sub-units. In this work, we focus on building up predictions about catalyst poisoning, from irreversible binding of the wrong substrate, and parasitic reduction channels, where charge is depleted reducing species other than oxygen, directly from density functional theory modeling of the binding of metalloporphyrin species to both the desired intermediates and a set of potential competing intermediates. Using these predictions as a baseline, we develop a machine learning model capable of generating this same information for novel electrocatalysts.