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Trends in Competing Oxygen and Chlorine Evolution Reactions over Electrochemically Formed Single-Atom Centers of MXenes

Single-atom catalysts (SACs) have been developed as a promising alternative for the design of highly active and selective catalysts, with experimental evidence confirming their successful synthesis. In a SAC catalyst, typically a transition metal – most commonly a precious metal – is embedded onto a support, and the resulting active site catalyzes chemical transformations relevant to energy conversion with high activity, selectivity, and maximum atomic efficiency. A typical selectivity problem encountered in the chemical industry refers to the competing oxygen (OER) and chlorine (CER) evolution reactions. While mixed-metal oxides, such as RuO2, IrO2, and TiO2, have been dominating the field of CER catalysis over the last 50 years, the selectivity of the competing reaction channels still imposes a challenge. [1-3]

Recent advances in SAC-based materials have revitalized this area of research by opening new avenues for the design of selective CER catalysts. While the recently synthesized SAC-based CER catalysts still rely on expensive platinum-group metals, low-cost alternatives based on earth-abundant elements have yet to be developed [4].

In this contribution, we demonstrate that SAC sites can also be formed electrochemically through water-mediated surface oxidation on the basal planes of MXenes, a class of two-dimensional materials composed of transition-metal carbides and nitrides [5]. Electrochemically formed SACs on MXenes could represent a promising alternative to CER catalysts as they eliminate the need for precious metals. By employing density functional theory (DFT) calculations combined with a descriptor-based analysis, we elucidate the relationship between in situ-formed SAC structures on MXenes and their catalytic performance in the competing oxygen (OER) and chlorine (CER) evolution reactions [6-7]. In total, 48 different SAC motifs are systematically screened to identify activity and selectivity trends in CER and OER. Our results highlight that group V-based MXenes (V2X, Nb2X, and Ta2X) as promising candidates for selective CER, thus providing first evidence that electrochemically formed SACs based on MXenes can be exploited as efficient catalytic materials for energy conversion and storage processes [8].

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