Platinum-Modified Cantor Alloys as High-Entropy Electrocatalysts for Oxygen Reduction Reaction

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High-entropy alloys (HEAs) have emerged as a promising discovery platform for the development of tunable catalyst materials.[1] Among these, the Cantor alloy (CrCoFeMnNi) has gained significant attention due to its composition of low-cost, earth-abundant elements. However, a significant challenge associated with the Cantor alloy is its susceptibility to degradation in acidic reaction environments.

To mitigate this issue, one strategy involves the incorporation of Platinum (Pt), a metal known for its high surface stability. In this study, we conduct an exhaustive computational screening of the CrCoFeMnNiPt composition space to enhance oxygen reduction reaction (ORR) catalytic activity, assuming the formation of a Pt skin due to surface reconfiguration (Figure 1a).[2]

This screening process is accomplished by introducing a correction to the existing workflow[3] to be able to work with monolayer models and to account for surface strain effects on the adsorption energies of *OH and *O species. This is a critical step as the adsorption energies are known to be influenced by the strain effects.

The comprehensive computational analysis within the CrCoFeMnNiPt composition space reveals that PtNi combination emerges as the optimal catalyst for ORR (Figure1b). This result aligns with experimental results[2], this suggests that the computational analysis method can pave the way for the development of more efficient and cost-effective ORR catalysts, thereby advancing the field of HEA research.

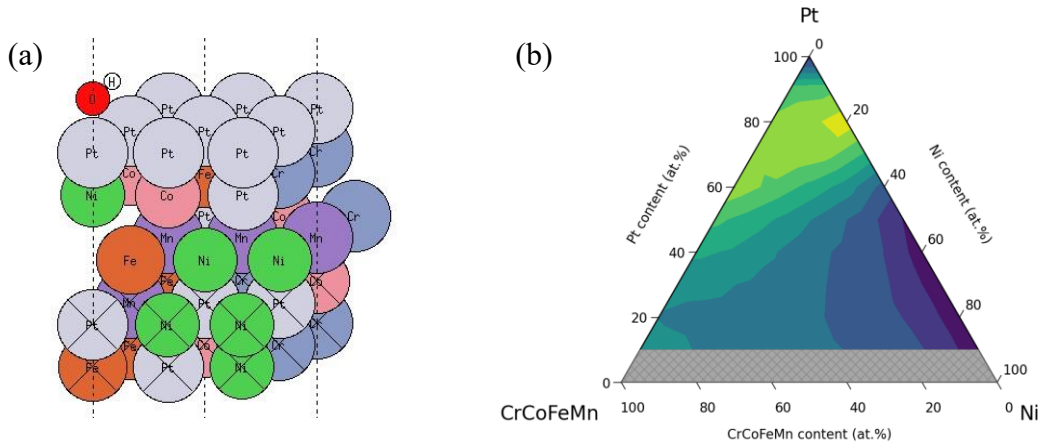

Figure 1: a) Example of a CrCoFeMnNiPt slab model. b) Ternary plot of oxygen reduction reaction activity for various Pt, Ni, and CrCoFeMn compositions, lighter colors represent more active compositions and darker colors indicate less active ones.

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