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# High through put screening of L12-type alloys: Proton-exchange membrane fuel cell application

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**The oxygen reduction reaction (ORR) has been considered as a critical bottle neck in development of proton-exchange membrane fuel cells (PEMFCs). The reaction has a relatively high over potential and its slow kinetics leads to main factor lowering power density. Above all, the usage of Pt, as an ORR catalyst, makes system price increase significantly and the catalyst degradation in the operating condition has been an important issue to solve. Therefore, it is highly required to develop new ORR catalyst which is cheap, highly durable and catalytically active for PEMFC commercialization. Here, we present the computational high through put screening of $L1_2$ alloy catalysts for developing ORR catalysts for PEMFC. It covers most of transition metals in periodic tables by setting the basic criteria such as heat of formation, O and OH adsorption energy and adsorption sites. While, we choose the ORR catalyst candidate, we consider not only catalytic activity but also the phase stability and price. After choosing the catalyst candidate, we studied the detailed reaction pathway to check into the validity of previous simple descriptor based screening study. From the density functional theory (DFT) calculations, we found that the new ORR catalyst has better catalytic activity both thermodynamically and kinetically compared to Pt. Based on various theory, we also considered the effective reversible potential and the cell efficiency to verify its catalytic performance.**

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