Prediction of Stable and Active (Oxy-Hydro) Oxide Nanoislands on Noble-Metal Supports for Electrochemical Oxygen Reduction Reaction

Developing cost-effective oxygen electrocatalysts with high activity and stability is key to their commercialization. However, economical earth-abundant catalysts based on first-row transition-metal oxides suffer from low electrochemical stability, which is difficult to improve without compromising their activity. Here, using density functional theory calculations, we demonstrate that noble-metal supports lead to bifunctional enhancement of both the stability and the oxygen reduction reaction (ORR) activity of metal (oxy-hydro) oxide nanoislands. We observe a significant stabilization of supported nanoislands beyond the intrinsic stability limits of bulk phases, which originates from a favorable lattice mismatch and reductive charge transfer from oxophilic supports. We discover that interfacial active sites (located between the nanoisland and the support) reinforce the binding strength of reaction intermediates, hence boosting ORR activity. Considering that both stability and activity lead to discovery of CoOOH|Pt, NiOOH|Ag, and FeO2|Ag as viable systems for alkaline ORR, we then use a multivariant linear regression method to identify elementary descriptors for efficient screening of promising cost-effective nanoisland|support catalysts.
Web of Science (2012): Impact factor 5.008
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 4.41 SJR 2.046 SNIP 1.404
Web of Science (2011): Impact factor 4.525
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 1.597 SNIP 0.944
Web of Science (2010): Impact factor 2.925
Web of Science (2010): Indexed yes
Web of Science (2009): Indexed yes
Original language: English
Keywords: Oxide, Oxy-hydroxide, FCC metal supports, Density functional theory calculations, oxygen reduction reaction, Pourbaix diagrams, Correlation analysis, Multivariant linear regression
DOIs:
10.1021/acsami.8b15428
Source: FindIt
Source-ID: 2442648205
Research output: Research - peer-review Journal article – Annual report year: 2019