High-Entropy Alloys as a Discovery Platform for Electrocatalysis

A theoretical method for finding active alloy electrocatalysts is proposed, and the method is applied to the electrochemical half-cell reaction of reducing oxygen to water, which is vital for improving the efficiency of, for example, hydrogen fuel cells. Our method predicts adsorption energies between reaction intermediates and the alloy surface to discover which sites on the surface are the most active. Starting from the multicomponent alloy IrPdPtRhRu, the alloy composition with best predicted catalytic activity is found.

General information
Publication status: Published
Organisations: Department of Energy Conversion and Storage, Atomic Scale Materials Modelling, Theoretical Atomic-scale Physics, Department of Physics, University of Copenhagen
Corresponding author: Rossmeisl, J.
Contributors: Batchelor, T. A., Pedersen, J. K., Winther, S. H., Castelli, I. E., Jacobsen, K. W., Rossmeisl, J.
Pages: 834-845
Publication date: 2019
Peer-reviewed: Yes

Publication information
Journal: Joule
Volume: 3
Issue number: 3
ISSN (Print): 1866-2021
Original language: English
Keywords: Electrocatalysis, ORR, High-entropy alloy, Multicompliment alloy, Machine learning, Rational-design
DOIs: 10.1016/j.joule.2018.12.015
Source: Scopus
Source-ID: 85062046208
Research output: Contribution to journal › Journal article – Annual report year: 2019 › Research › peer-review