Computational Study of Nb-Doped-SnO2/Pt Interfaces: Dopant Segregation, Electronic Transport, and Catalytic Properties - DTU Orbit (07/08/2019)

Carbon black, a state-of-the-art cathode material for proton exchange membrane fuel cells (PEMFCs), suffers from severe corrosion in practical applications. Niobium-doped tin dioxide (NTO) is a promising alternative to support the Pt catalysts at the cathodes. Here, through a combined density functional theory and non equilibrium Green's function study, we investigate the Nb segregation at Pt/NTO interfaces under operational electrochemical conditions, and reveal the resulting effects on the electronic transport, as well as the catalytic properties. We find that the Nb dopants tend to aggregate in the subsurface layers of the NTO substrate, whereas their transport across the Pt/NTO interface is hindered by a high thermodynamic barrier under the operating condition of PEMFCs. The interfacial transport of Sn is, however, more facile, indicating possible formations of Sn Pt alloys and tin oxides. The electronic conductivities of the Pt/NTO systems are not particularly sensitive to the distance of the Nb dopants relative to the interface, but depend explicitly on the Nb concentration and configuration. Through a dopant induced ligand effect, the NTO substrates can improve the catalytic activity of the Pt adsorbate toward the oxygen reduction reaction. We also investigate the co-doped SnO2 substrates by both Nb and Sb elements, and find that a small amount of Nb dopants could further improve the electronic transport of the Pt/Sb-doped-SnO2 interface. The fundamental understanding generated here will help shed light on future applications of Nb-doping and Nb-Sb co-doping in Pt/SnO2 type cathodes for PEMFC applications.

General information
Publication status: Published
Organisations: Atomic Scale Materials Modelling, Department of Energy Conversion and Storage
Pages: 1641-1649
Publication date: 2017
Peer-reviewed: Yes

Publication information
Journal: Chemistry of Materials
Volume: 29
Issue number: 4
ISSN (Print): 0897-4756
Ratings:
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 9.74 SJR 4.675 SNIP 1.893
Web of Science (2017): Impact factor 9.89
Web of Science (2017): Indexed yes
Original language: English
DOIs:
10.1021/acs.chemmater.6b04879
Source: FindIt
Source-ID: 2352293075
Research output: Contribution to journal › Journal article – Annual report year: 2017 › Research › peer-review