Decoupling Strain and Ligand Effects in Ternary Nanoparticles for Improved ORR Electrocatalysis - DTU Orbit (03/12/2018)

Decoupling Strain and Ligand Effects in Ternary Nanoparticles for Improved ORR Electrocatalysis

Density functional theory is used to investigate OH adsorption on ternary Pt-Au-M (M = 3d-metal) nanoparticles in order to address their potential to improve activity for the oxygen reduction reaction (ORR) compared to pure Pt nanoparticles. The nanoparticles are investigated through a method developed for decoupling strain and ligand effects and then correlated with the extended Pt(111) surface for benchmarking. Subsurface Au has previously been shown to form a passivating layer, stabilising the nanoparticle catalysts against the harsh acidic conditions at the cathode, while the current study shows the effect of the ternary metal core allowing for tuning the catalytic activity through strain effects. Good agreement is found with experimental studies showing increased activity of Pt-Au-Fe/Ni nanoparticles, and the current study suggests that mid to late 3d-metals should also exhibit enhanced activity and stability with respect to pure Pt nanoparticles. It is suggested that the Pt-Au-M for M = Cr, Mn, Co, Cu, Zn nanoparticles are of particular interest as they exhibit an optimal interplay between strain, ligand effects and stability.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Number of pages: 9
Pages: 24737-24745
Publication date: 2016
Peer-reviewed: Yes

Publication information

Journal: Physical Chemistry Chemical Physics
Volume: 18
ISSN (Print): 1463-9076
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.04 SJR 1.686 SNIP 1.089
Web of Science (2017): Impact factor 3.906
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.06 SJR 1.685 SNIP 1.113
Web of Science (2016): Impact factor 4.123
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.45 SJR 1.725 SNIP 1.205
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.29 SJR 1.771 SNIP 1.239
Web of Science (2014): Impact factor 4.493
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 4.05 SJR 1.72 SNIP 1.207
Web of Science (2013): Impact factor 4.198
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.67 SJR 1.921 SNIP 1.177
Web of Science (2012): Impact factor 3.829
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.6 SJR 1.707 SNIP 1.19