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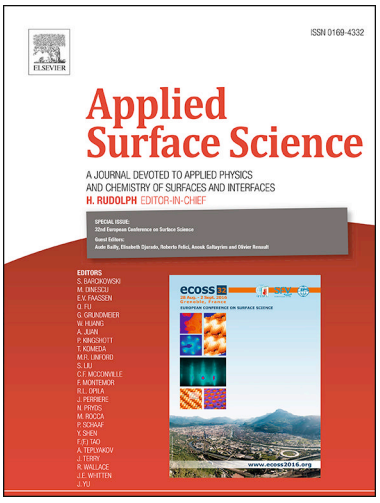

Full Length Article

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PII: S0169-4332(18)32462-0
DOI: https://doi.org/10.1016/j.apsusc.2018.09.045
Reference: APSUSC 40349

To appear in: *Applied Surface Science*

Received Date: 26 February 2018
Revised Date: 18 August 2018
Accepted Date: 5 September 2018

Please cite this article as: Y. Nan, Y. Wang, D. Cao, Y. Yang, D. Cheng, Adsorption and Dissociation of Borohydride on Different Ir-Ni Alloy Surfaces, *Applied Surface Science* (2018), doi: https://doi.org/10.1016/j.apsusc.2018.09.045

Adsorption and Dissociation of Borohydride on Different Ir-Ni Alloy Surfaces

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Abstract

Borohydride (BH_4^-) is considered as one of promising hydrogen storage materials, which could serve as hydrogen source for proton exchange membrane fuel cells (PEMFCs). In this study, the adsorption and dissociation of BH_4^- on seven Ir-Ni alloy surfaces are investigated by density functional theory (DFT) calculations. Our results indicate that the doping proportion of Ir atoms on these surfaces can affect the adsorption configurations of BH_{4ad}. The $1Ir_2Ni$-2Ir-Ni(111) surface (Ni(111) with surface Ir_2Ni and subsurface Ir) has been found as the most beneficial one for the dissociation of BH_{4ad} among these systems. Moreover, the influence of water molecules is discussed. It is found that the binding energies of BH_{4ad} for all systems would decrease by the presence of H_2O molecules, due to the reduced charge transfer of B atom and H atoms in BH_{4ad}. In addition, the adsorption of OH_{ad} would weaken the effect of H_2O molecules for BH_{4ad} hydrolysis on all alloy surfaces. It is expected that our results can provide useful insights for the design and development of Ir-Ni catalysts for borohydride hydrolysis.

Keywords: borohydride hydrolysis, Ir-Ni bimetallic catalysts, density functional theory calculations

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