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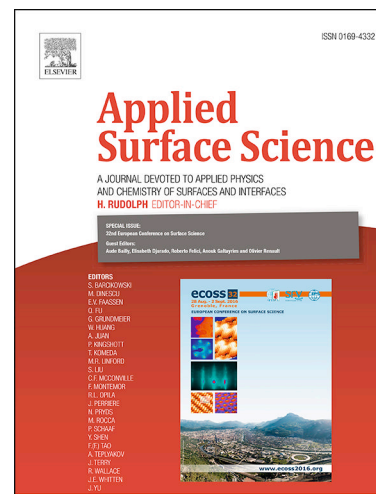
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Adsorption and Dissociation of Borohydride on Different Ir-Ni Alloy Surfaces

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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 $\text{BH}_{4\text{ad}}$. The 1Ir₂Ni-2Ir-Ni(111) surface (Ni(111) with surface Ir₂Ni and subsurface Ir) has been found as the most beneficial one for the dissociation of $\text{BH}_{4\text{ad}}$ among these systems. Moreover, the influence of water molecules is discussed. It is found that the binding energies of $\text{BH}_{4\text{ad}}$ for all systems would decrease by the presence of H₂O molecules, due to the reduced charge transfer of B atom and H atoms in $\text{BH}_{4\text{ad}}$. In addition, the adsorption of OH_{ad} would weaken the effect of H₂O molecules for $\text{BH}_{4\text{ad}}$ 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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