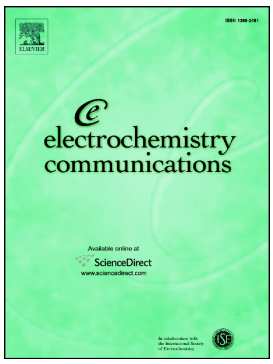

Hydrogen adsorption in the presence of coadsorbed CO on Pd(111)

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Hydrogen adsorption in the presence of coadsorbed CO on Pd(111)

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Abstract

Carbon monoxide is related to many catalytic processes and it is necessary to understand the effects that arise by the influence of this specie in the electronic structure of the material surface. In this study we performed DFT calculations to investigate the coadsorption of hydrogen and carbon monoxide on the Pd(111) surface. We determined the adsorption energy of hydrogen in the presence of pre-adsorbed CO to be 0.11 eV lower in comparison to a bare palladium surface, suggesting that even in small amounts this molecule can block active sites.

Keywords: carbon monoxide, hydrogen adsorption, density functional theory, electrocatalysis

1. Introduction

Using density functional theory (DFT) researchers have been able to perform electronic structure calculations accurately and efficiently until certain detail of surface chemical properties [1]. To understand surface chemical reactivity and catalysis (surface chemical properties) is fundamental to describe the chemical bond between a surface and a molecule [2]. DFT-based models have been largely used in the past of few decades for micro-kinetic modeling, computational catalysts screening, and reaction mechanism discovery [3].

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