

平成 19 年 10 月 29 日

応用物理学会北海道支部
会員各位

応用物理学会北海道支部

講演会のお知らせ

下記講演会を開催いたしますので、多数ご参加下さいますようご案内申し上げます。

演題：Oxygen Adsorption on the Ir(111): A First Principle Study

講師：Hong Zhang 氏

(School of Physical Science and Technology, Sichuan University , China /
Associate professor)

日時：平成 19 年 11 月 8 日 (木) 13:30 ~ 15:00

場所：北海道大学 創成科学研究棟 4 階 セミナー室 A

主催：応用物理学会北海道支部

講演の要旨

As a late 5d transition metal, Iridium shows potential in a great variety of applications, particularly as an effective heterogeneous catalyst in various industrial chemical reactions, and the structure sensitive reactions on its surface is important in many catalytic reactions, Ir and Ir-alloy catalysts are widely used in reactions that require the activation of C-H bonds. It is also considered as an improvement to the automobile catalytic converter because of its unique ability to decompose NO as well as reduce NOx in the presence of hydrocarbons. Clearly it would be valuable to have a detailed atomic-level understanding of these reactions which could lead to the designing of Ir-based catalysts with greater selectivity and activity.

I will report my recent studies ---investigating oxygen adsorption on the Ir(111) by using first-principle method. We present ab initio calculations for atomic oxygen adsorption on Ir(111) for a wide range of oxygen coverages, and focus on the (111) surface and present results for oxygen adsorption and the initial oxidation, and determine the pressure-temperature phase diagram for conditions extending from ultra high vacuum to those typical of technical catalysis and compare the results to other O/TM systems.

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