



## Energy related processes on metal oxide surfaces

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表面科学およびナノサイエンス、特に酸化物表面研究の分野において、走査プローブ顕微鏡等を用いた研究展開で著名な Thornton 先生が来日される機会に、本学にてセミナーをお願いいたしました。聴講を歓迎いたします。

Two topics will be covered in this talk. The first is related to the fact that metal oxides form a large body of active catalysts and catalyst supports, with  $\text{CeO}_2$  and  $\text{TiO}_2$  being important examples. Corresponding characterisation of model single crystal surfaces have played a pivotal role in understanding the basic physics and chemistry that underpin their remarkable properties. Attention has recently turned towards single atom catalysis as a means of enhancing catalytic activity and reducing the use of expensive supported metals. This talk will examine the potential of polaron manipulation by materials design to position metal atoms. I will compare the adsorption of single gold atoms on  $\text{CeO}_2(111)$  and  $\text{TiO}_2(110)$ . The former substrate can be O terminated by atoms bound to three Ce atoms in the layer below. It can also be terminated by  $\text{Ce}=\text{O}$ . In both cases gold atoms are bound to O atoms and not to O vacancies as predicted by DFT. This differs from the behaviour on  $\text{TiO}_2(110)$ , where Au atoms are bound to vacancies. These findings are explained by the polaronic nature of the Au- $\text{CeO}_2$  system, which modifies the diffusion characteristics of the Au atoms from those encountered on  $\text{TiO}_2$ .

The second topic is associated with the discovery that semiconducting oxides such as ZnO and  $\text{TiO}_2$  can photocatalytically split water. There has been a huge effort to increase the efficiency of the process as a means of harnessing solar energy. Most of this work has involved empirical testing, although there has been a significant amount of surface science aimed at understanding the detailed mechanism. More recently, this has been extended to in-situ measurements at liquid-solid interfaces. This talk will describe our current understanding of the crystallography of the interface between  $\text{TiO}_2$  and liquid electrolytes. Remarkably, these interfaces are characterized by an ordering of the contact layer. For instance, chlorine and hydroxyls are ordered in the contact layers of oxide aqueous interfaces, with implications for the photo-physics and chemistry.

連絡教員 物理学系 斎藤 晋 (内線 2070)