

FeO Interaction with Water from UHV Condition to Ambient and in Electrolyte

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Iron oxides are promising catalysts in various reactions for energy conversion and storage such as the HER, the OER, etc. The adsorption and dissociation of water plays a central role since the energetics of water interaction with catalytic sites is fundamental to regulate both activity and selectivity. We prepared model systems of FeO ultrathin films on Au(111) and investigated by STM and XPS, their interaction with water vapors under UHV conditions, at ambient pressure and in alkaline electrolyte.

Submonolayer of FeO were deposited on the Au(111) surface (figure 1a) according to a previous recipe.^[1] The as-prepared surface was exposed at RT to water vapors showing a “pressure gap” in dissociative chemisorption, being necessary to reach a rather elevated pressure (mbar range) to detect the finger print of hydroxyls in the XPS O 1s. The STM images showed very bright areas with a similar periodicity of FeO/Au(111) Moiré (3.3 nm). The inset of figure 1b shows a high-resolution image that allow to discern highly dense bright spots, clustering on the FCC regions of FeO/Au(111) surface.^[2] Moreover, by comparing series of images acquired at successive times, it was possible to deduce a fast diffusion and high mobility of such OH species.^[3] The stability of FeO-OH_x films in the ambient air was proved by both the STM images (see figure 1c) and O 1s photoemission spectra (figure 1h). Then we proceeded our investigation and used the EC-STM to monitor the FeO_x in 0.1 M KOH. Figure 1d-f were the sequence of atomically resolved images acquired from -110 mV to 150 mV (vs RHE), where the FeO is stable. We observed the diffusion and disappearance of bright protrusions, suggesting that in alkaline solution the FeO surface is partially populated by mobile OH species.

Our study indicates that FeO/Au(111) is capable of dissociating water and the resulting FeO-OH_x films is stable at room temperature. The in-situ measurement in electrolyte paves the ways for further operando study and a better understanding of the HER reaction.

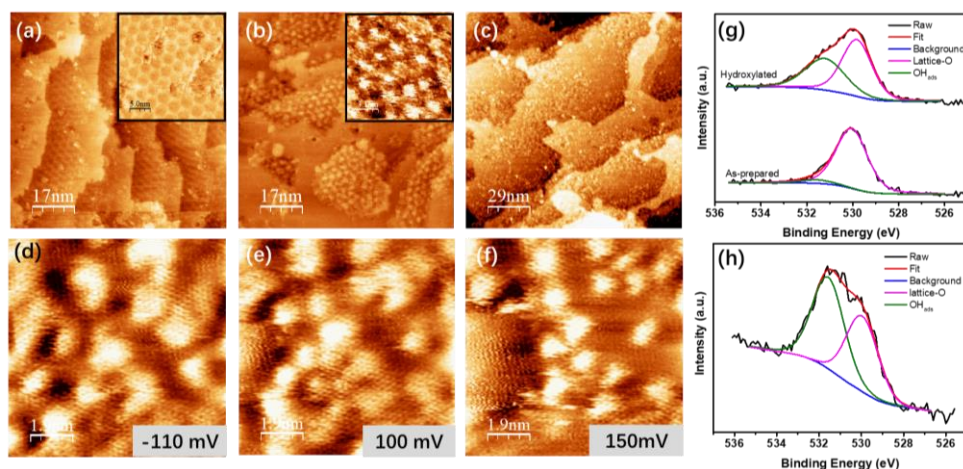


Fig. 1. The STM image of (a) 0.5 ML FeO on Au(111), FeO-OH_x/Au(111) (b) in UHV and (c) in Air. (d-f) The consecutive images of FeO_x/Au(111) in 0.1 M KOH. The XPS of (g) FeO, FeO-OH_x and (h) FeO-OH_x after air exposure.

[1] Merte, L. R, *et al.*; Nat Commun **5**, 4193 (2014)

[2] Li, Y *et al.*; ACS Nano **13**, 11632-11641 (2019)

[3] Sun, Z *et al.*; J Phys Condens Matter **34**, 16 (2022)