

Hematite photoanode bifunctionalization through modification with ytterbium and molybdenum

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Photoelectrochemical water splitting has attracted significant attention as a method to convert solar light into a clean and renewable fuel. Since the first demonstration of photoelectrochemical water splitting using TiO₂^[1], a large number of semiconductor materials have been studied as photoelectrodes. Among the different semiconductor materials, hematite is a promising candidate as a photoanode because of its stability, abundance, low cost and favorable band gap.^[2,3] However, its performance is limited because of the poor conductivity and extremely short carrier diffusion length, which implies significant electron-hole recombination.^[2]

Here, we present a novel procedure to bifunctionalize hematite through modification with ytterbium and molybdenum. Both modifications were done by an impregnation method (drop-casting). We found that the addition of only ytterbium passivates the surface states of hematite for efficient solar water splitting, while the addition of only molybdenum increases the electron concentration.^[3] The modification was sequential, beginning either with Mo or Yb. The obtained results reveal a sensitivity to the order in which the modifiers are introduced (Figure 1). When the modification of hematite was carried out adding first ytterbium followed by the addition of molybdenum their effects are roughly additive (see blue curves in Figure 1). In contrast, if the modification of hematite is carried out adding first molybdenum followed by the addition of ytterbium, the effects are synergetic (see pink curves in Figure 1).

It is worth noting that in both cases the bifunctionalization of hematite with ytterbium and molybdenum is achieved, leading to an enhancement of the photoresponse of the pristine material. Interestingly, both Mo and Yb seem to preserve their separate roles in the bifunctionalized samples.

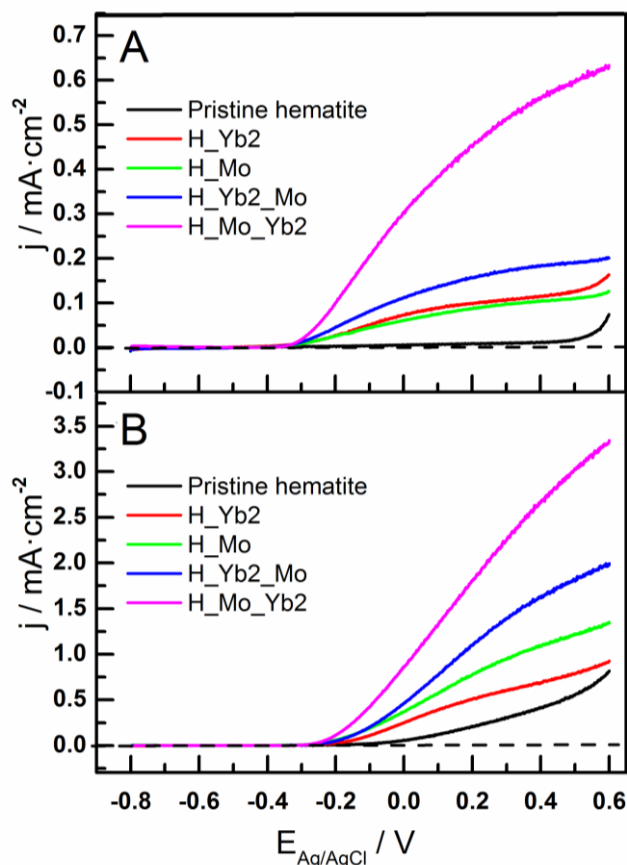


Figure 1. Current density vs potential measured in N_2 -purged aqueous 1M NaOH. (a) linear voltammograms obtained under EE illumination ($250 \text{ mW}\cdot\text{cm}^{-2}$, $\lambda > 350 \text{ nm}$) and (b) linear voltammograms obtained under SE illumination ($250 \text{ mW}\cdot\text{cm}^{-2}$, $\lambda > 350 \text{ nm}$) for pristine hematite (black), hematite modified with ytterbium (H_Yb2, red), hematite modified with molybdenum (H_Mo, green), hematite modified with ytterbium first and molybdenum (H_Yb2_Mo, blue) and hematite modified with molybdenum first and ytterbium (H_Mo_Yb2, pink).

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References:

- [1] A. Fujishima, K. Honda. *Nature*, **1972**, 238, 37
- [2] K. Sivula, F. Le Formal, M. Grätzel. *ChemSusChem*, **2011**, 4, 432
- [3] A. Cots, D. Cibrev, P. Bonete, R. Gómez. *ChemElectroChem*, 10.1002/celec.201600644