

Characterization of Sb_2Se_3 single crystal surfaces for photocatalysis

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Solar light-driven water oxidation and reduction are achieved, in photoelectrochemical cells (PEC), by utilizing semiconductor materials as photoelectrodes. Thus, in order to realize low-cost, commercialized PEC, the employment of appropriate inexpensive, easily fabricated semiconductors is mandatory.

Sb_2Se_3 is, in this context, a promising photoelectrode. In fact, its constituents are both earth-abundant and relatively cheap. It is a binary chalcogenides, allowing a much simpler control over its phase and defects, with respect to other multinary chalcogenides [1]. It has a direct band gap of 1.0-1.2 eV, with a high optical absorption coefficient [2]. Moreover, it shows a peculiar crystalline structure with parallel-stacked 1D ribbons (Fig. 1a) whose edges are occupied by saturated atoms, minimizing recombination losses [3]. Therefore, it assures efficiency in visible-infrared light absorption and subsequent electron-hole separation. Furthermore its conduction band minimum, located at -4.15 eV [4], makes it a good photocathode for hydrogen evolution reaction.

We studied cleaved Sb_2Se_3 samples realizing a complete ultra-high vacuum surface science characterization. By means of XPD and LEED we determined the surface orientation of the crystal as (100). STM directly showed 1D ribbons (Fig. 1b). The band structure and band bending profile at the semiconductor surface were studied with ARPES and angle-resolved XPS, respectively. This allowed us to obtain information on the electronic properties, fundamental in view of a possible implementation of Sb_2Se_3 as a PEC electrode material.

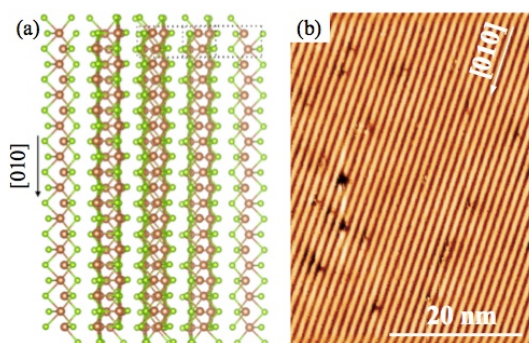


Figure 1: Schematic representation (a) and STM image (b) of parallel-stacked Sb_2Se_3 1D ribbons. Image conditions: 35 nm x 50 nm, $V_{\text{sample}} = 1.4$ V, $I_{\text{tunnel}} = 190$ pA.

References

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