Enhanced photoelectrochemical performance of tungsten oxide film by bifunctional Au nanoparticles

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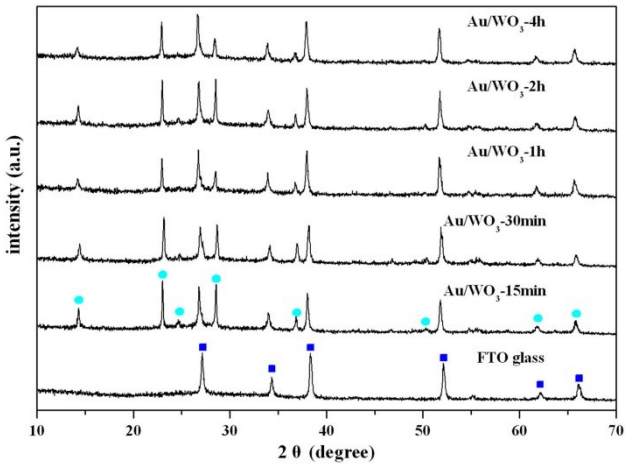

S1. X-ray diffraction (XRD) patterns for the Au/WO_3-X samples.

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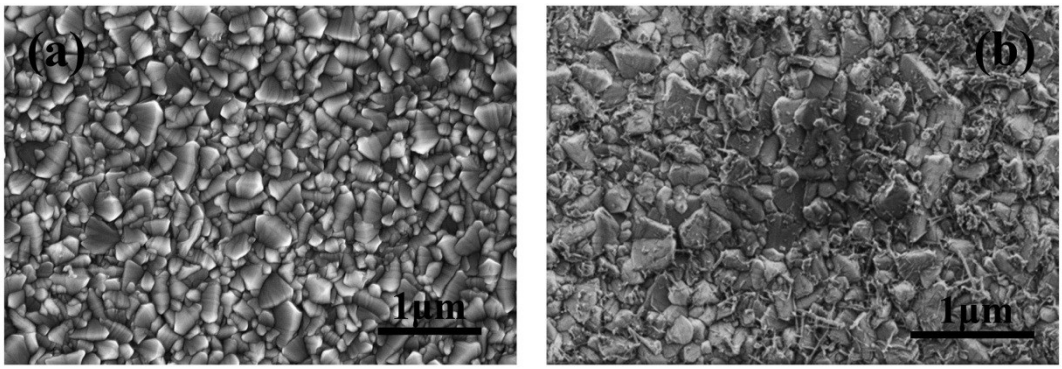
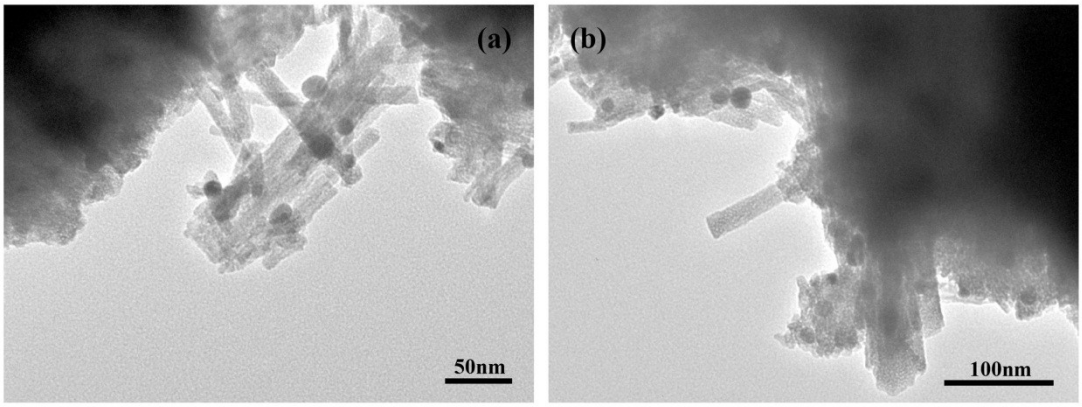
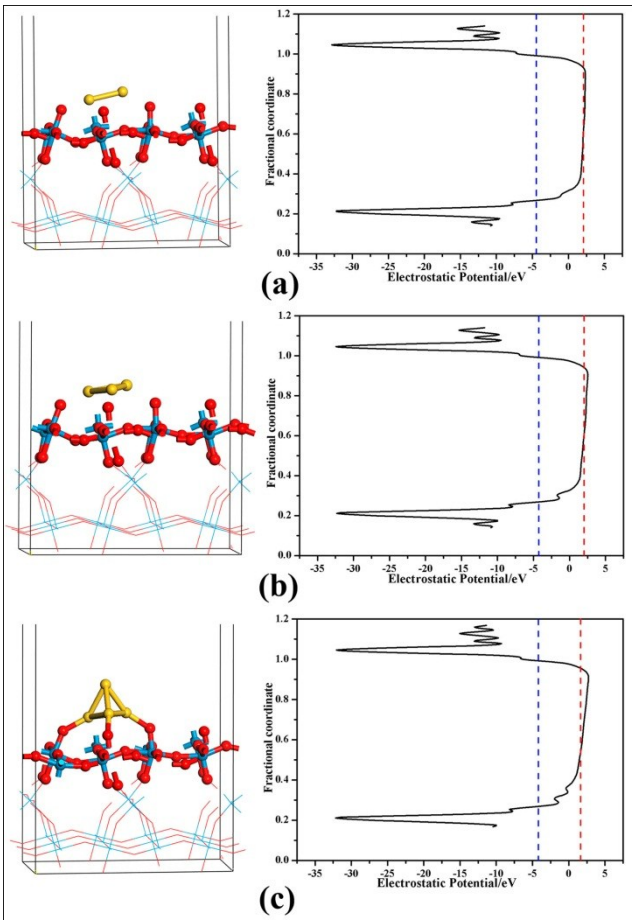


S2. Top-view SEM images of (a) the bare FTO glass and (b) the FTO glass with crystal seed.



S3. The HRTEM of (a) Au/WO_3-2h and (b) Au/WO_3-4h samples. The diameter of the Au nanoparticles are about 25nm.



S4. The surface structures (left) and potentials (right) for WO_3 (010) face with (a) two, (b) three, and (c) four Au atoms. The calculated work functions for the three models are 6.71, 6.06, and 5.57 eV.

Theoretical parameters

Density functional theory (DFT) calculations were performed using Cambridge Sequential Total Energy Package (CASTEP). The generalized gradient approximation

(GGA) with the Perdew-Burke-Ernzerhof (PBE) functional was used for the exchange and correlation interactions. The ultrasoft pseudopotential was used to deal with the core electrons and the valence electrons are O $2s^2 2p^4$, W $5s^2 5p^6 5d^4 6s^2$, and Au $5d^{10} 6s^1$. The hexagonal WO_3 crystal cell with P6/MMM space group was completely relaxed in the present work. To achieve the accurate lattice parameters, the plane wave cutoff was set as 340.0 eV, and the k-point of 2×2×4 was used for the relaxation using the Monkhorst-Pack scheme. All forces on atoms were converged to less than 0.03 eV/Å, the maximum ionic displacement was within 0.001 Å, and the total stress tensor was reduced to the order of 0.05 GPa. The optimized lattice parameters were a=b=7.454Å and c=3.830Å, in good agreement with the experimental value of a=b=7.298 Å, and c=3.899Å. The WO_3 (010) surfaces without/with Au atoms were modeled using the relaxed crystal cell. The models consisted of (2×2) unit cell with seven atom layers and a 30 Å vacuum layer. The above models were fully relaxed using k-points of 2×2×1.