Supporting Information

The effects of crystal structure and electronic structure on photocatalytic H_2 evolution and CO_2 reduction over two phases of perovskite-structured $NaNbO_3$

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SI-1 The catalysts characterizations before and after H_2 evolution and CO_2 reduction

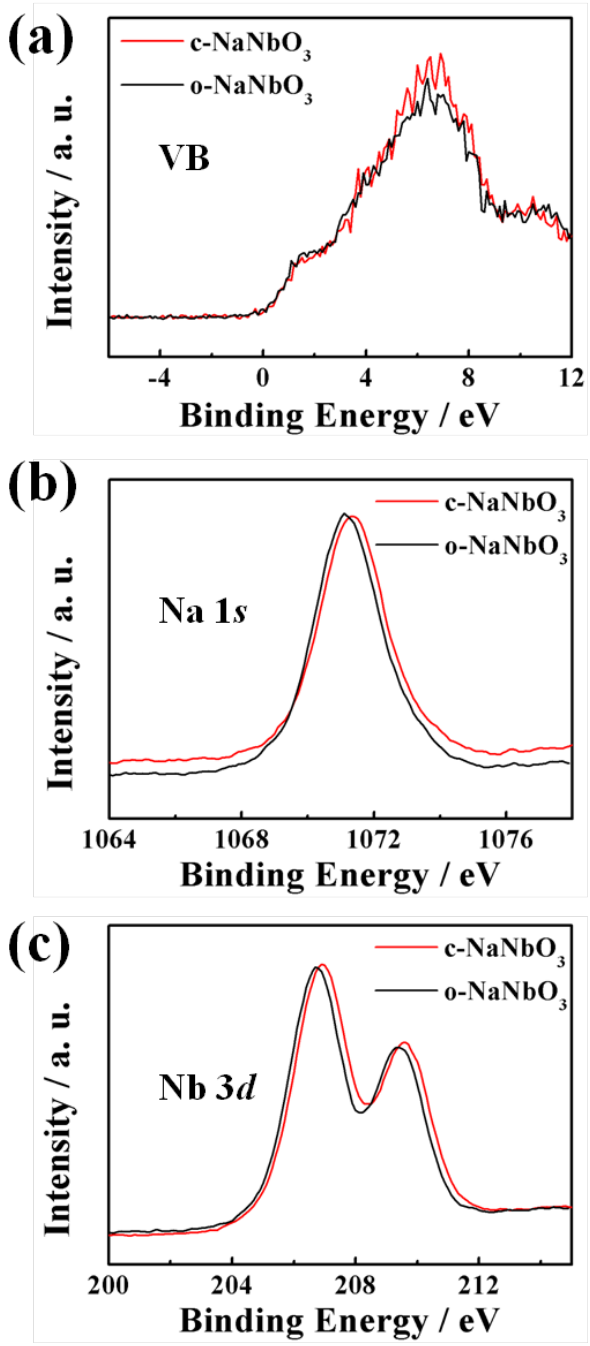

Figure S1. The XPS spectra of the as-prepared $NaNbO_3$ samples. (a) Valence bands (VB) of c-$NaNbO_3$ and o-$NaNbO_3$. (b) Na 1*s* of c-$NaNbO_3$ and o-$NaNbO_3$. (c) Nb 3*d* of c-$NaNbO_3$ and o-$NaNbO_3$.

The XPS spectra results in Figure S1 indicate the valence band, Na 1*s* and Nb 3*d* energy levels of c-$NaNbO_3$ and o-$NaNbO_3$. In Figure S1(a), the same valence band energy level suggests that the valence band tops have the same energy which is also proved by the theoretical calculation. In Figure S1(b) and S1(c), the energy levels of Na 1*s* and Nb 3*d* electrons increase 0.3 eV and 0.2 eV respectively from c-$NaNbO_3$ to o-$NaNbO_3$. This phenomenon indicates that the electronic structures of two $NaNbO_3$ samples are different, and the theoretical energy levels of Na 1*s* and Nb 3*d* orbitals (supplied in Figure S3) lend support to such difference between cubic and orthorhombic $NaNbO_3$.

SI-2 The catalysts characterizations before and after H_2 evolution and CO_2 reduction

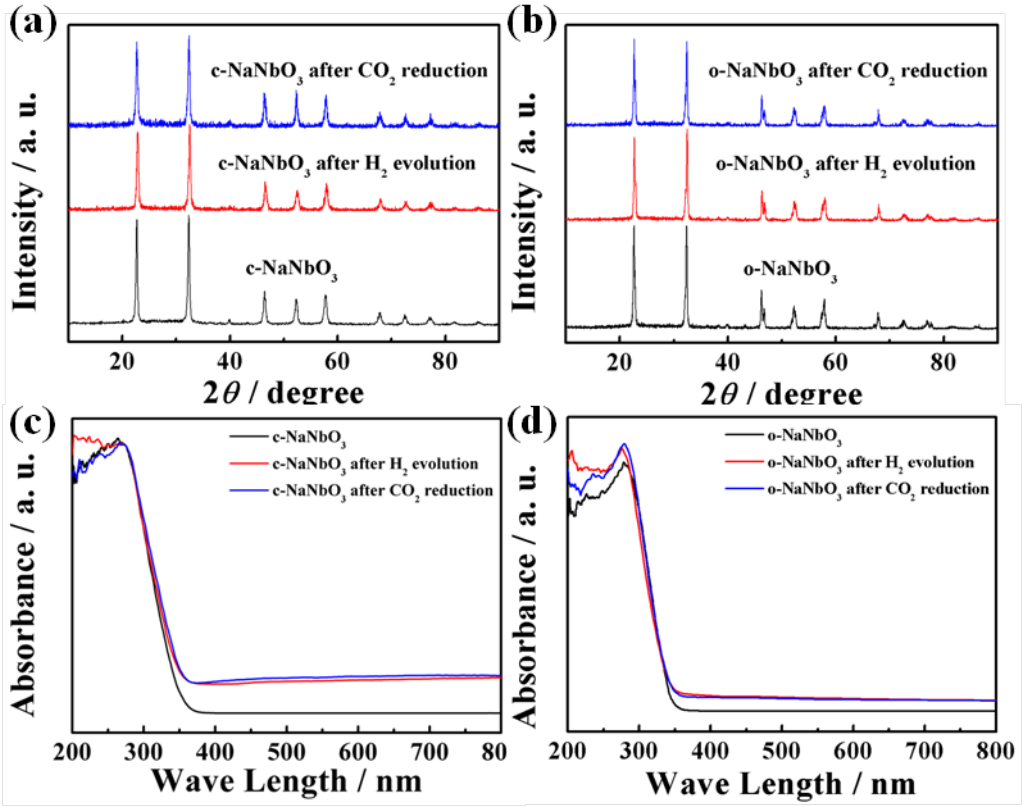

Figure S2. (a) XRD patterns of original c-$NaNbO_3$ and c-$NaNbO_3$ after H_2 evolution and CO_2 reduction. (b) XRD patterns of original o-$NaNbO_3$ and o-$NaNbO_3$ after H_2 evolution and CO_2 reduction. (c) UV-visible sbsorption spectra of original c-$NaNbO_3$ and c-$NaNbO_3$ after H_2 evolution and CO_2 reduction. (d) UV-visible sbsorption spectra of original o-$NaNbO_3$ and o-$NaNbO_3$ after H_2 evolution and CO_2 reduction.

SI-3 Partial density of states (PDOS) of Nb 3*d* and Na 1*s* orbitals

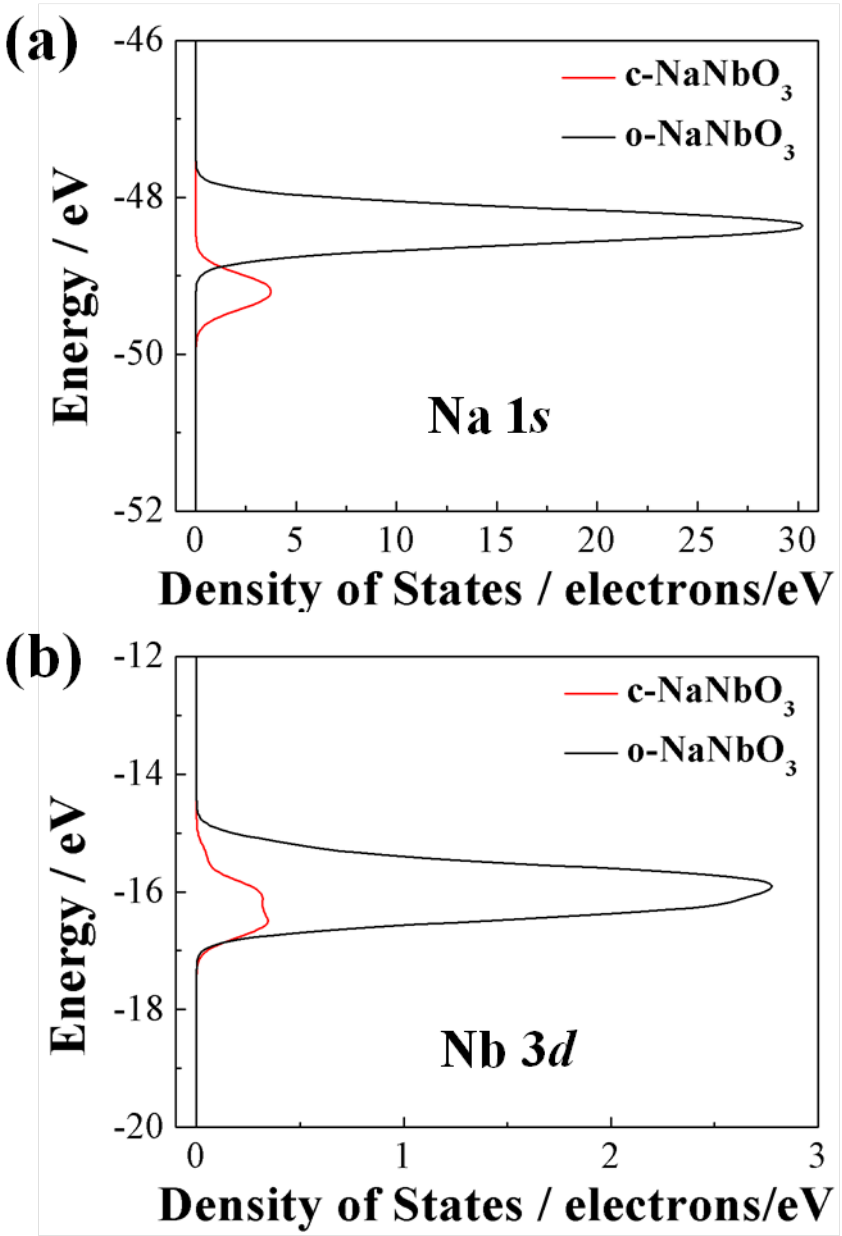

Figure S3. (a) PDOS of Na 1*s* orbital. (b) PDOS of Nb 3*d* orbital.