Supplementary Information

Energetic stability and photocatalytic activity of $SrTiO_3$ nanowires: *Ab initio* simulations

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The band structures of both non-stoichiometric and stoichiometric $SrTiO_3$ nanowires in the vicinity of the energy gaps $\Delta\varepsilon_{gap}$ between the tops of the valence band (VB) and the bottoms of the conduction band (CB) or the Fermi levels (E_F) have been calculated using the hybrid DFT-LCAO *PBE0* method within the formalism of the localized atomic orbitals [1]. The band structures of non-stoichiometric 4×4 STO NWs with SrO and TiO_2 terminations are shown in Figs. *SI*1a,b, respectively. In both cases, the bottoms of the CBs are crossed by the Fermi levels.

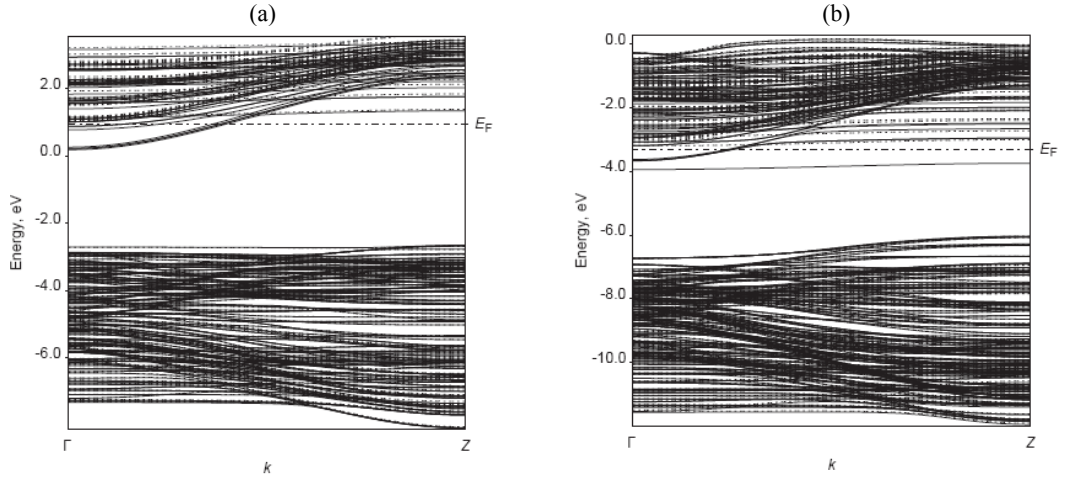

Figure SI1. Electronic band structure of non-stoichiometric 4×4 $SrTiO_3$ nanowires along the ***k*** vector with overall symmetric: (a) SrO-termination and (b) TiO_2-termination.

Obviously, the band structures of non-stoichiometric NWs obtained in the current study can be described as non-direct since the CB bottom is achieved at Γ point of the BZ, whereas the VB top corresponds to Z point for both terminations, analogously to Ref. [2].

Analogously to both types of non-stoichiometric nanowires, the band gaps of stoichiometric nanowires (Fig. *SI*2) remain non-direct since the CB bottom is achieved at Γ point of the Brilluoin zone (BZ), whereas the VB top corresponds to Z point. Values of $\Delta\varepsilon_{gap}$ are noticeably smaller than those for TiO_2-terminated $SrTiO_3$ nanowires and markedly smaller as compared to SrO-terminated STO NWs when comparing those for similar values of d_{NW}:

$$\Delta\varepsilon_{gap}^{stoichiometric} < \Delta\varepsilon_{gap}^{TiO_2\_non\text{-}stoichiometric} < \Delta\varepsilon_{gap}^{SrO\_non\text{-}stoichiometric}.$$

The widths of band gaps of both non-stoichiometric and stoichiometric STO nanowires consequently decrease with growing values of d_{NW} for the same NW morphology.

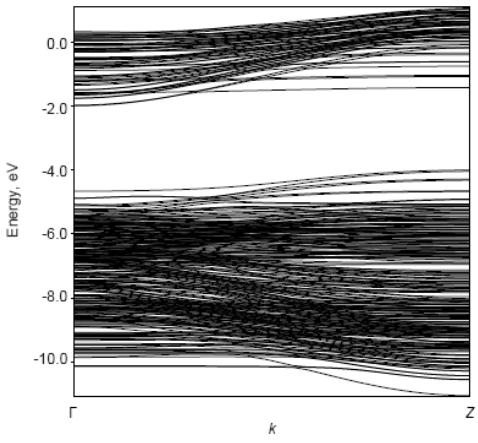

Figure SI2. The electronic band structure of stoichiometric 5×5 $SrTiO_3$ nanowire along the ***k*** vector.

[1] C. Adamo and V. Barone, *J. Chem. Phys.* **110**, 6158 (1999).
[2] Q. Fu, T. He, J.L. Li, and G.W. Yang, *J. Appl. Phys.* **112**, 104322 (2012).

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