## Supplementary Information

## Energetic stability and photocatalytic activity of SrTiO<sub>3</sub> 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<sub>2</sub> terminations are shown in Figs. *SI*1a,b, respectively. In both cases, the bottoms of the CBs are crossed by the Fermi levels.



*Figure SII*. Electronic band structure of non-stoichiometric  $4 \times 4$  SrTiO<sub>3</sub> nanowires along the *k* vector with overall symmetric: (a) SrO-termination and (b) TiO<sub>2</sub>-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  $\Gamma$  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  $\Gamma$  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<sub>2</sub>terminated SrTiO<sub>3</sub> nanowires and markedly smaller as compared to SrO-terminated STO NWs when comparing those for similar values of  $d_{NW}$ :

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

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



*Figure SI2.* The electronic band structure of stoichiometric  $5 \times 5$  SrTiO<sub>3</sub> nanowire along the *k* vector.

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