

**SUPPLEMENTARY MATERIALS for:**

**Vitamin C Affinity to TiO<sub>2</sub> Nanotubes:  
A Computational Study by Hybrid Density Functional Theory  
Calculations**

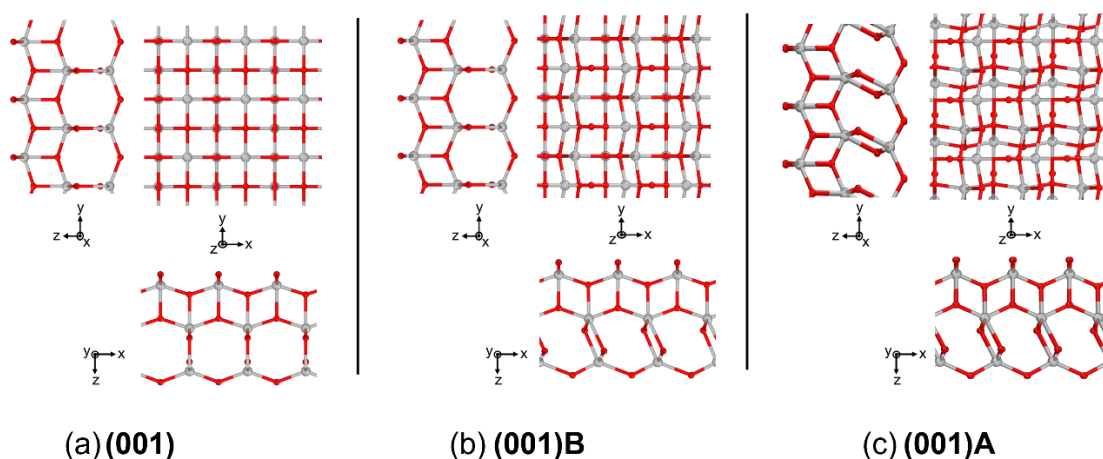
Aldo Ugolotti,<sup>a</sup> Mirko Dolce,<sup>a</sup> Cristiana Di Valentin<sup>a,b,\*</sup>

<sup>a</sup> Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, via R. Cozzi 55, 20125 Milano, Italy

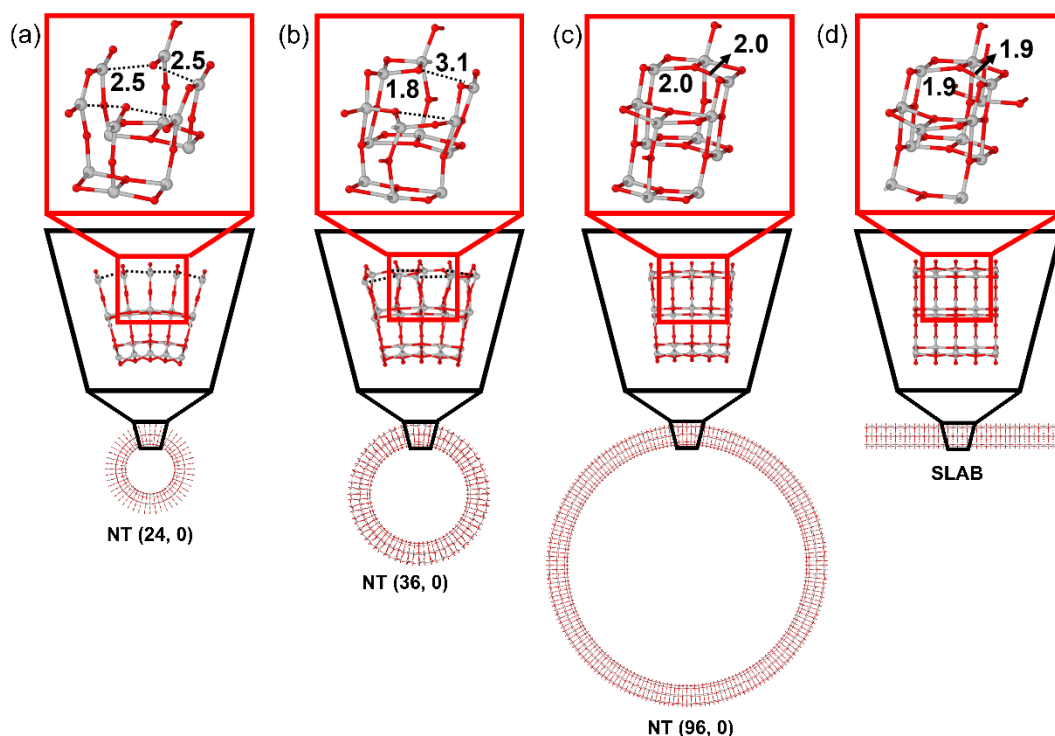
<sup>b</sup> BioNanoMedicine Center NANOMIB, Università di Milano-Bicocca, via R. Follereau 3, 20854 Veduggio al Lambro, Italy

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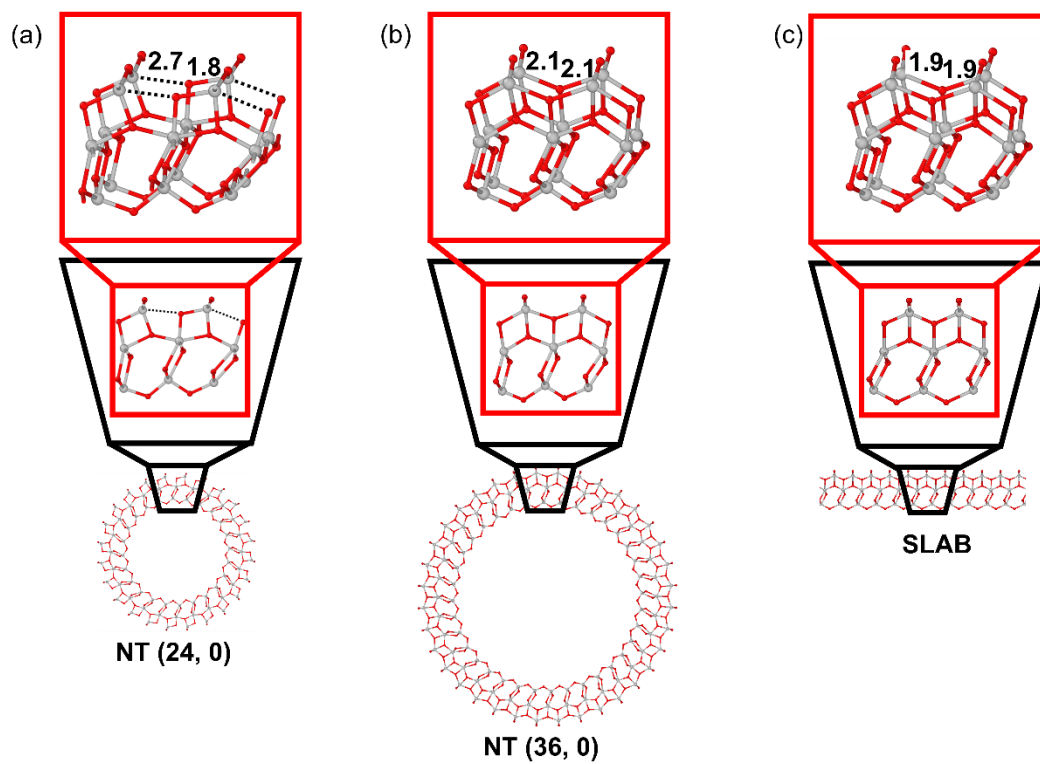
\* Corresponding author: cristiana.divalentin@unimib.it



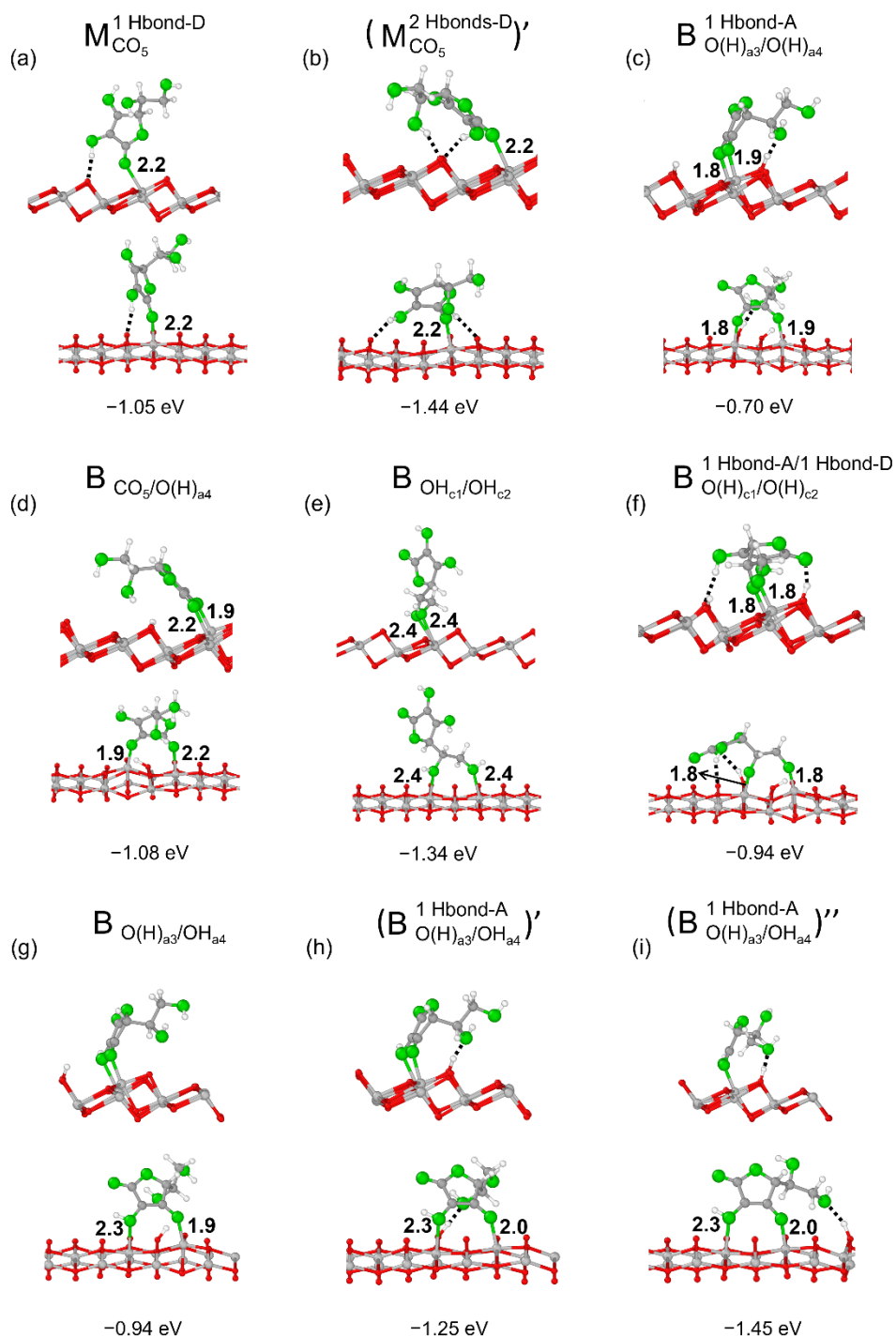
**Figure S1:** Structure of  $\text{TiO}_2$  3L slabs for the (001) (panel a), (001)B (panel b) and (001)A (panel c) surfaces. Surface (001)B can be constructed through a rigid shift of the highest triatomic layer along the x direction. Surface (001)A is obtained with an additional shift of the lowest triatomic layer along the  $-y$  direction [Ref.: Ferrari et al., J. Phys. Chem. Lett. 1, 19, 2854–2857 (2010)]. Each panel reports a top view and the side views along [010] and [100] crystallographic directions. Ti and O atoms are represented with light grey and red spheres, respectively.



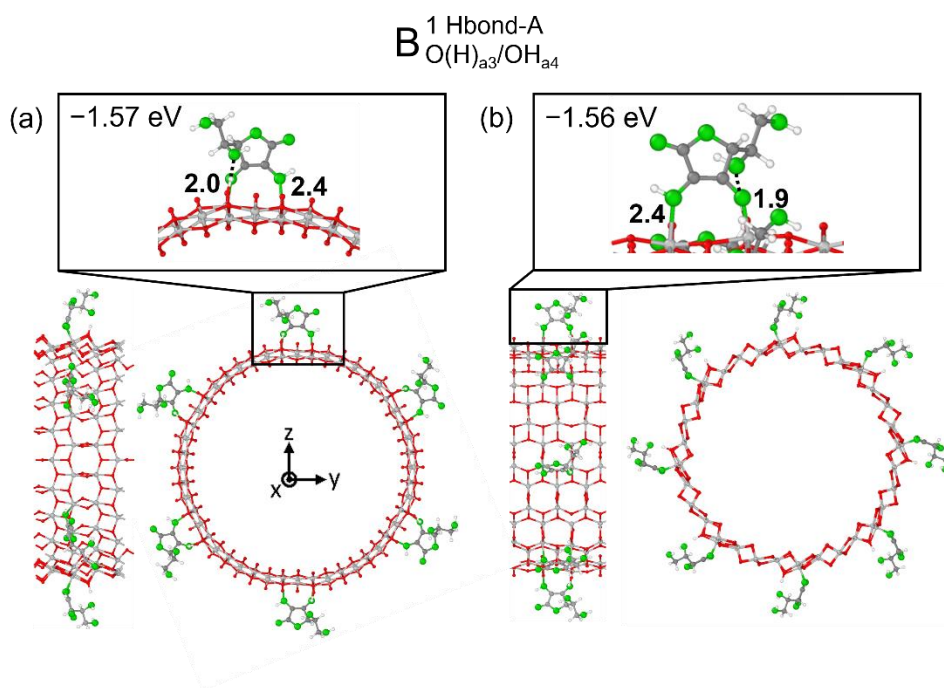
**Figure S2:** Structure of  $\text{TiO}_2$  NT (101) 3L with different diameters and of the related flat (101) surface. Each panel includes two different views of the structure; dashed black lines mark the broken bonds. Ti and O atoms are represented with light grey and red spheres, respectively. Relevant distances are reported in Å.



**Figure S3:** Structure of  $\text{TiO}_2$  NT (001)A 3L with different diameters and of the related flat (001)A surface. Each panel includes two different views of the structure; dashed black lines mark the broken bonds. Ti and O atoms are represented with light grey and red spheres, respectively. Relevant distances are reported in Å.



**Figure S4:** Adsorption configurations and energies per molecule ( $\Delta E_{\text{ads}}^{\text{mol}}$ ) of additional optimized models of Vitamin C on the  $\text{TiO}_2$  (101) 1L surface (panels a-i). Panels g, h and i report models that differ in the position of the transferred proton. In each panel, the top/bottom image reports the side view along the [010]/[10-1] crystallographic direction. Ti, C, H atoms are represented with light grey, dark grey and white spheres, respectively. Oxygen atoms of Vitamin C/slab are represented with green/red spheres. Solid and dashed black lines mark the electrostatic and hydrogen bonds, respectively. Relevant distances are reported in Å.



**Figure S5:** Optimized configurations and adsorption energies per molecule ( $\Delta E_{\text{ads}}^{\text{mol}}$ ) for a single adsorption mode of Vitamin C on different  $\text{TiO}_2$  NT (101) 1L configurations. In panel a the NT is constructed with a (24, 0) roll-up index while in panel b with a (0, 24) index.

In each panel, the left/right image reports the front/side view while on top a zoom on the molecule is shown. Ti, C, H atoms are represented with light grey, dark grey and white spheres, respectively. Oxygen atoms of vitamin C/slab are represented with green/red spheres. Solid and dashed black lines mark the electrostatic and hydrogen bonds, respectively. Relevant distances are reported in Å.