Supplementary Information for

Electronic and optical properties of TiO_2 nanotubes and arrays: A first-principles study

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We perform test calculation for electronic structures of TiO_2 monolayer, bilayer, and bulk at the HSE06, PBE, and DFT+U levels. These predicted band gaps are summarized in Table S1.

Table S1 The predicted band gaps (in eV) of TiO_2 monolayer, bilayer and bulk at the HSE06, PBE, and DFT+U levels.

TiO_2	HSE	PBE	Shear facter	DFT+U
monolayer	4.27	2.76	1.51	3.86
bilayer	4.12	2.66	1.46	3.77
bulk	3.29	1.92	1.37	3.26

As examples, by using the PBE and HS06 functionals, and DFT+U method, we carry out additional calculations for band structures of TiO_2 bilayer, as shown in Fig. S1. The calculated results show that the band structures of TiO_2 sheets can be well described by using PBE functional. As shown in Figure S1, a shear factor of 1.51 eV is needed to obtain the reliable band gap, compared with the corresponding HSE06 results. Note that we do not obtain the reliable conduction bands of TiO_2 bilayer by using DFT+U method.

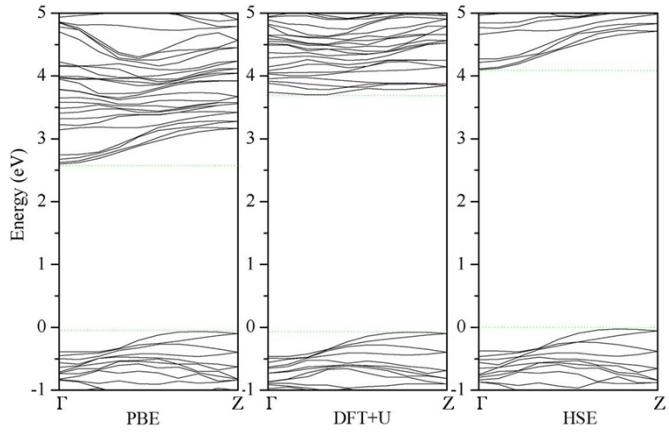

Fig. S1 Band structures of TiO_2 bilayer at the PBE, DFT+U and HSE06 levels.

The optimized D_{4d} and S_8 (-4, 4) SWTONTs are plotted in Figs. 1(b) and 1(c), respectively. Clearly, they display polygon- and circle-like configurations, as shown in Fig. S2.

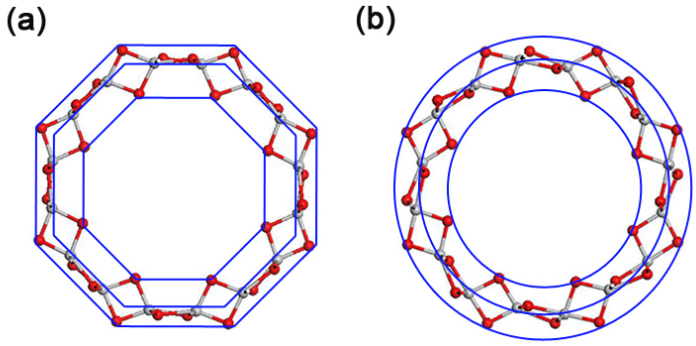

Fig. S2 Optimized structures. (a) Polygon-like D_{4d} (-4, 4) SWTONT, (b) Circle-like S_8 (-4, 4) SWTONTs.