

Supplementary Information

Geometric and electronic properties of the ultrathin anatase TiO_2 (001) films

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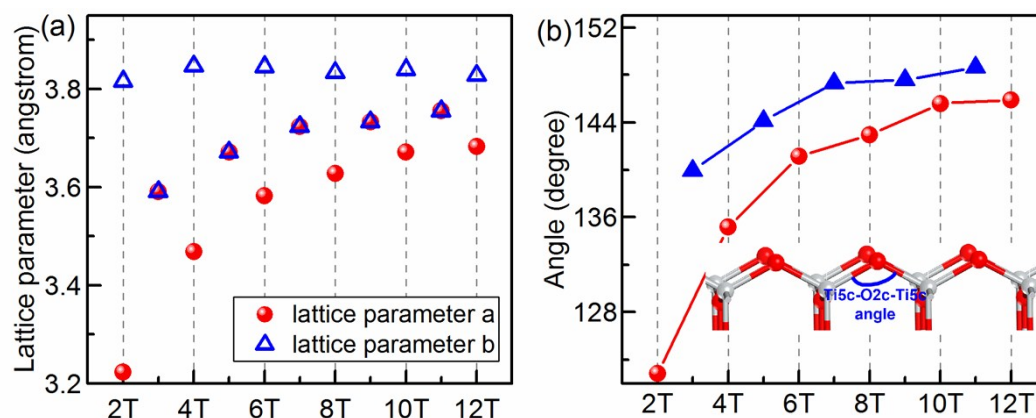


Figure S1. Calculated (a) lattice parameters and (b) surface Ti5c-O2c-Ti5c angles with the PBE-D2 functional. The films with 2 to 12 trilayers are denoted respectively by 2T to 12T.

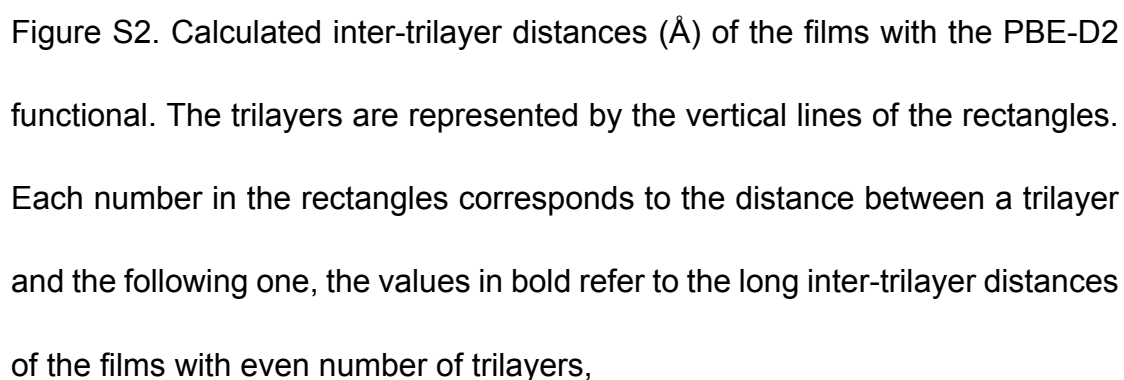


Figure S2. Calculated inter-trilayer distances (Å) of the films with the PBE-D2 functional. The trilayers are represented by the vertical lines of the rectangles. Each number in the rectangles corresponds to the distance between a trilayer and the following one, the values in bold refer to the long inter-trilayer distances of the films with even number of trilayers,