

## **Electronic Supplementary Information (ESI)**

### **Surface-Functionalized Monolayered Nanodots of a Transition Metal Oxide and Their Properties**

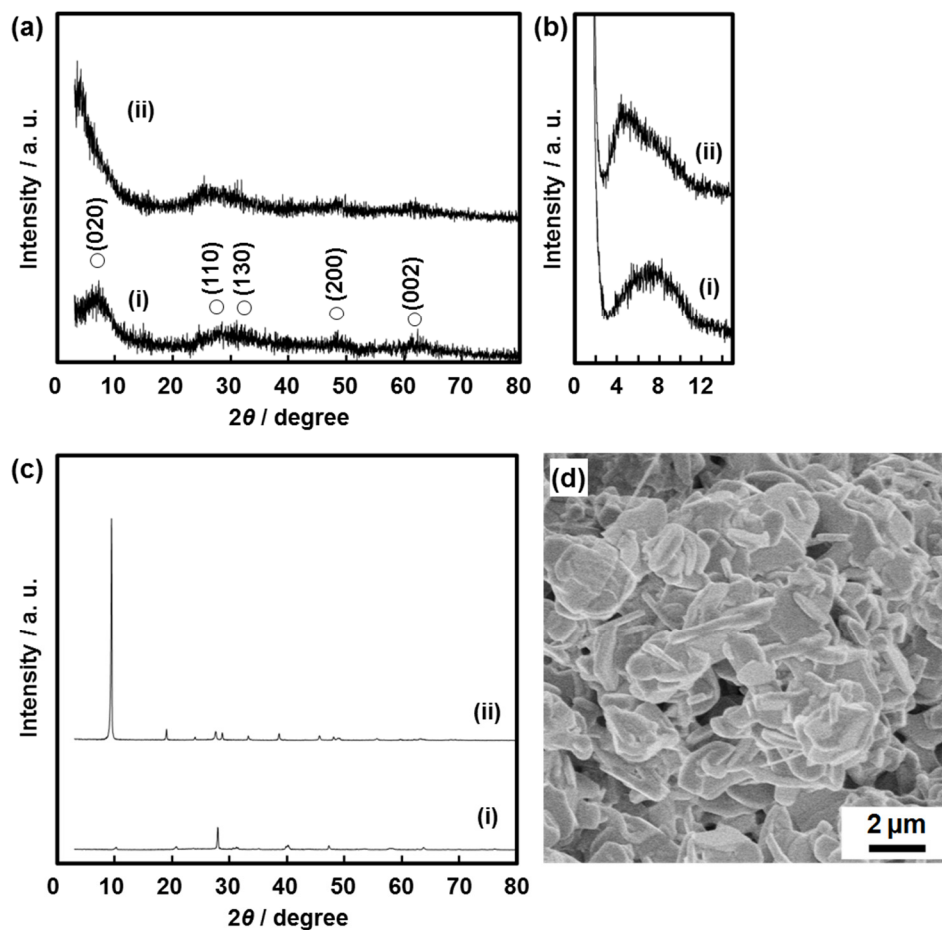
Masashi Honda, Yuya Oaki,\* Hiroaki Imai\*

Department of Applied Chemistry, Faculty of Science and Technology, Keio University, 3-14-1 Hiyoshi, Kohoku-ku, Yokohama 223-8522, Japan

#### **Contents**

Structures of the precursor layered titanates (Fig. S1)	P. S2
UV-Vis spectra of the $\mu\text{m-TiO}_2$ and $\text{nm-TiO}_2$ (Fig. S2)	P. S3

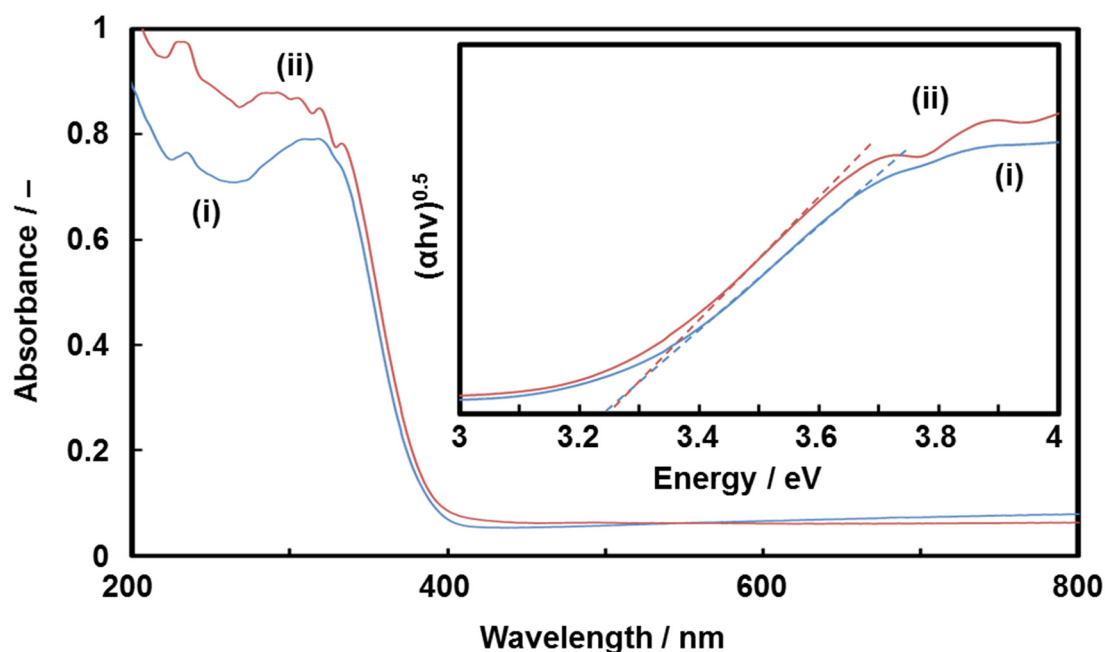
## Structures of the precursor layered titanates



**Fig. S1** XRD patterns (a,b) and FESEM images (c,d) of the precursor nanocrystals (a,b) and bulk crystals (c,d). In the panels (a,b), the spectra (i) and (ii) correspond to the Na-TiO<sub>2</sub> nanocrystals and H-TiO<sub>2</sub> after the protonation, respectively. In the pane (c), the spectra (i) and (ii) correspond to the bulk Cs-TiO<sub>2</sub> crystals and H-TiO<sub>2</sub> after the protonation, respectively.

The interlayer distances, namely those of the (020) planes, were shifted after the ion-exchange from the alkaline ions to proton (Fig. S1a,c).

## UV-Vis spectra of the $\mu\text{m-TiO}_2$ and $\text{nm-TiO}_2$



**Fig. S2** UV-Vis spectra and their Tauc's plots (the inset) of the  $\text{nm-TiO}_2$  (i) and  $\mu\text{m-TiO}_2$  (ii).

The  $E_g$  of the  $\mu\text{m-TiO}_2$  and  $\text{nm-TiO}_2$  2–5 nm in size was estimated to be  $E_g=3.24$  eV and  $E_g=3.25$  eV, respectively. As mentioned in the main text, the effect of the lateral size reduction is calculated to be  $\Delta E_{g,\text{calc.}}=0.019\text{--}0.12$  eV by the first term of the (eq. 1) on the assumption of  $L_{x,y}=2.0\text{--}5.0$  nm and  $\mu_{x,y}=1.63m_e$  as the reduced effective mass of bulk anatase titanium dioxide. In the present work, the experimental  $E_g$  of the  $\text{nm-TiO}_2$  would have the slight deviations because of the reproducibility of size distribution and crystallinity resulting from the solution syntheses.