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

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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$_2$ nanocrystals and H-TiO$_2$ after the protonation, respectively. In the pane (c), the spectra (i) and (ii) correspond to the bulk Cs-TiO$_2$ crystals and H-TiO$_2$ 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 μm-TiO₂ and nm-TiO₂

Fig. S2  UV-Vis spectra and their Tauc’s plots (the inset) of the nm-TiO₂ (i) and μm-TiO₂ (ii).

The $E_g$ of the μm-TiO₂ and nm-TiO₂ 2–5 nm in size was estimated to be $E_{g\text{,μm}}=3.24$ eV and $E_{g\text{,nm}}=3.25$ eV, respectively. As mentioned in the main text, the effect of the lateral size reduction is calculated to be $\Delta E_{g,\text{calc.}}=0.019–0.12$ eV by the first term of the (eq. 1) on the assumption of $L_{x,y}=2.0–5.0$ 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 nm-TiO₂ would have the slight deviations because of the reproducibility of size distribution and crystallinity resulting from the solution syntheses.