Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information for

Liquid Exfoliation of Five-Coordinated Layered Titanate $K_2Ti_2O_5$ Single Crystals in Water

Fumitaka Hayashi,[†,‡,] Kenta Furui,[†] Nanako Tatewaki,[†] Tomohito Sudare,[§] Maru Kashiwazaki,[†] Hiromasa Shiiba,[§] Hideki Tanaka,[§] Michihisa Koyama,[§] Chiaki Terashima,[§,#] and Katsuya Teshima[†,‡,§,#,]**

[†]Department of Materials Chemistry, Faculty of Engineering, Shinshu University, 4-17-1 Wakasato, Nagano 380-8553, Japan

[‡]Global Aqua Innovation Center, Shinshu University, Wakasato, Nagano 380-8553, Japan

[§]Research Initiative for Supra-Materials (RISM), Shinshu University, 4-17-1 Wakasato, Nagano 380-8553, Japan

[#]Research Center for Space System Innovation, Tokyo University of Science, 2641 Yamazaki, Noda, 278-8510, Japan

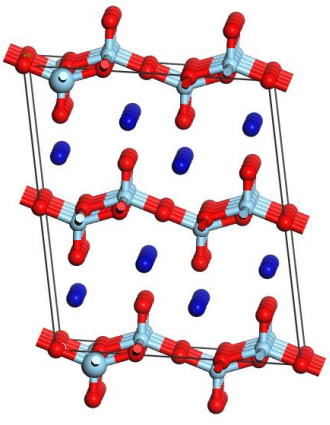
* Corresponding author, fhayash@shinshu-u.ac.jp; teshima@shinshu-u.ac.jp.

Table S1. Immersion Effect in Solvents on Exfoliation of Layered Titanate $K_2Ti_2O_5$ Crystals

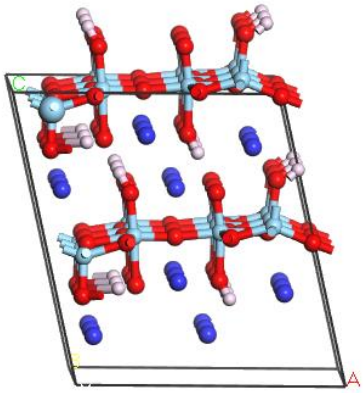
Entry	Solvent	Tyndall scattering
1	$CHCl_3$	X[a]
2	$C_2H_5OC_2H_5$	X[a]
3	$C_6H_5CH_3$	X[a]
4	Diethyl carbonate $C_5H_{10}O_3$	X[a]
5	Ethylene carbonate (EC), $C_3H_4O_3$	X[a]
6	*N*,*N*-dimethylformamide (DMF) $(CH_3)_2NCHO$	X[a]
7	Dimethyl sulfoxide (DMSO) C_2H_6SO	X[a]
8	*N*-methylpyrrolidone C_5H_9NO	X[a]
9	Acetone CH_3COCH_3	✓
10	Ethanol C_2H_5OH	X[a]
11	Acetic acid CH_3COOH	X[a]
12	Tetrahydrofuran (THF) C_4H_8O	X[a]
13	Water H_2O	✓

[a] Tyndall scattering is not confirmed.

(a)



(b)



(c)

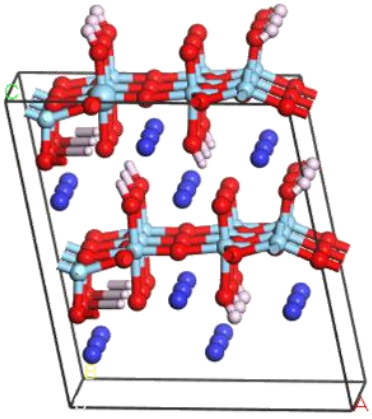


Figure S1. Core-hole positions of (a) $K_2^{[5]}Ti_2O_5$, (b) $K_2^{[6]}Ti_2O_5$-H_2O, and (c) $K_2^{[5]}Ti_2O_5$-H_2O. Sample abbreviation is the same as those in the main text. Blue, light blue, red, and pink spheres represent K, Ti, O, and H, respectively. Large light blue balls in the figures indicate the core-hole positions for the Ti species.

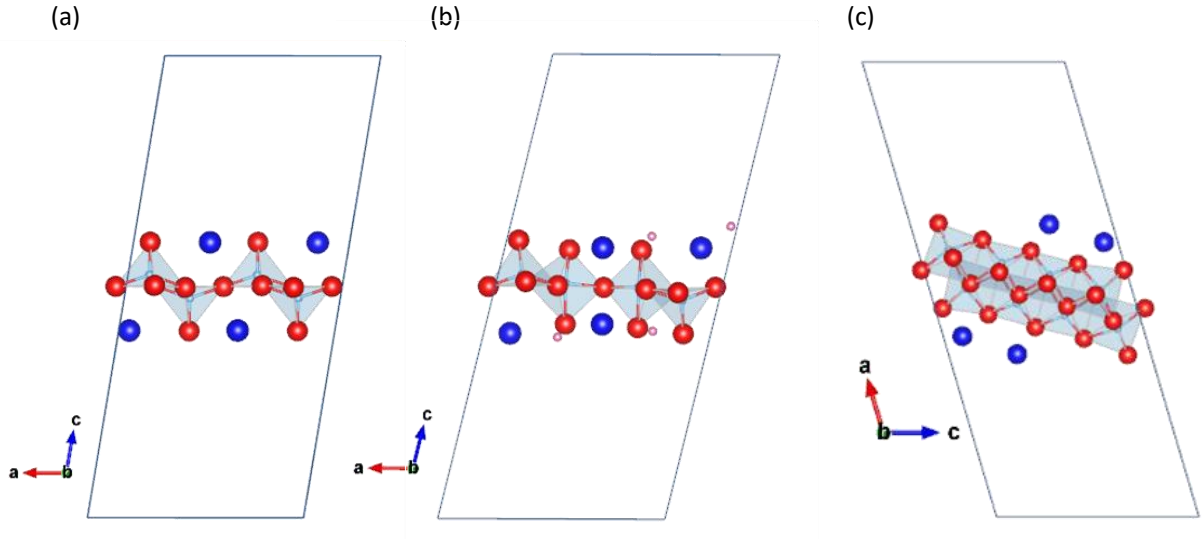


Figure S2. Slab models of (a) $K_2Ti_2O_5$, (b) $K_2Ti_2O_5$-H_2O, and (c) $K_2Ti_4O_9$ for exfoliation energy calculation. Blue, light blue, red, and pink spheres represent K, Ti, O, and H, respectively.

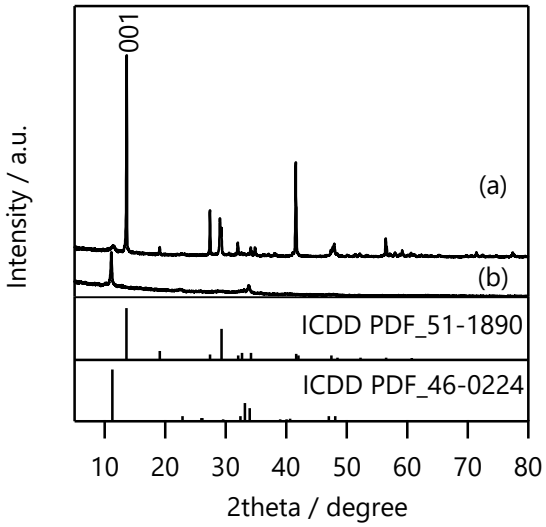


Figure S3. XRD patterns of (a) parent $K_2Ti_2O_2$ crystals and (b) $K_2Ti_2O_2$ crystals after the storage in 1 day under ambient conditions together with those of the references $K_2Ti_2O_5$ (PDF 51-1890) and $K_2Ti_2O_5 \cdot nH_2O$ (PDF 46-0224).

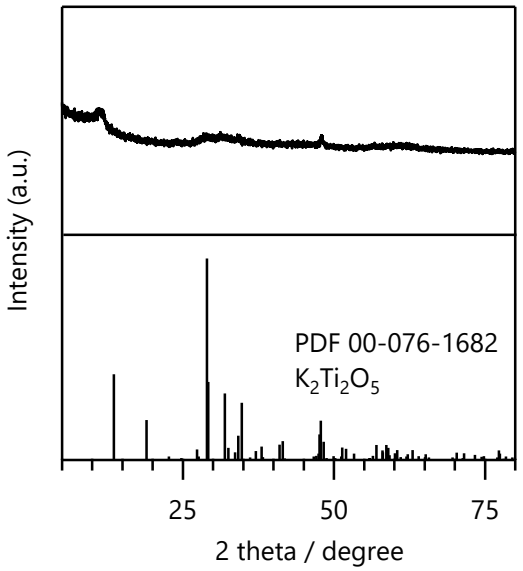


Figure S4. XRD pattern of titanate nanosheet precipitate after the hydrothermal treatment.

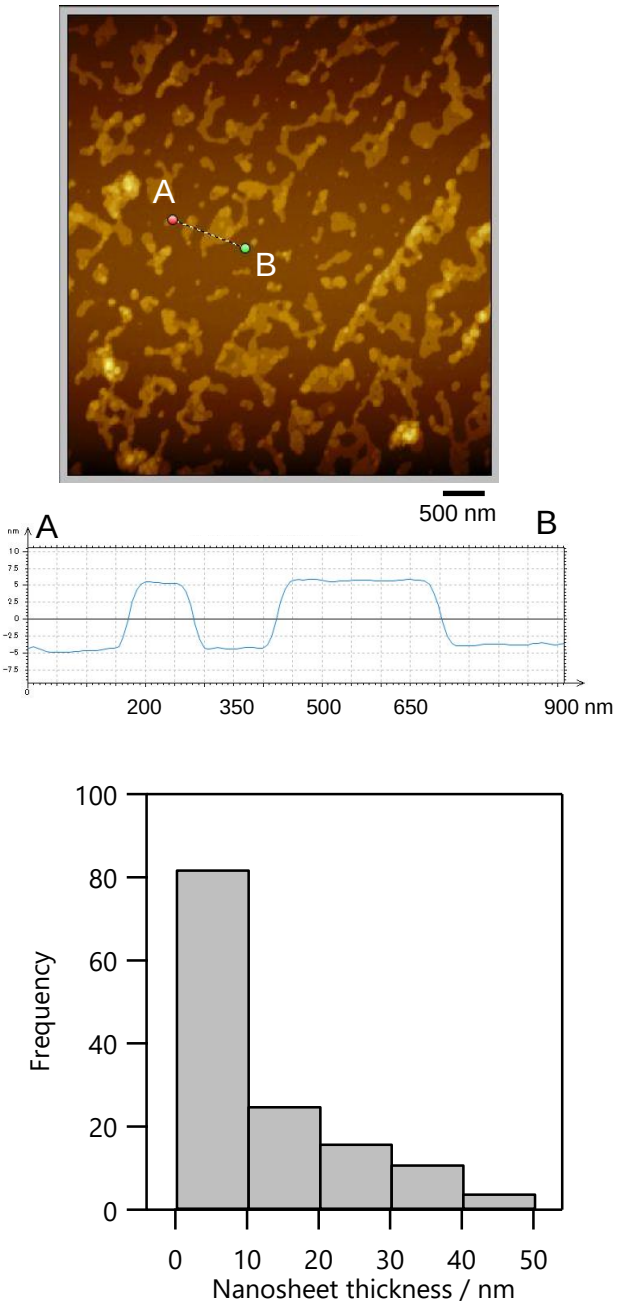


Figure S5. (Top) AFM image of the $K_2Ti_2O_5$ sample prepared by dispersing the colloidal nanosheet suspension on a Si surface. (Bottom) statistical distribution results on the KTO nanosheet thickness.

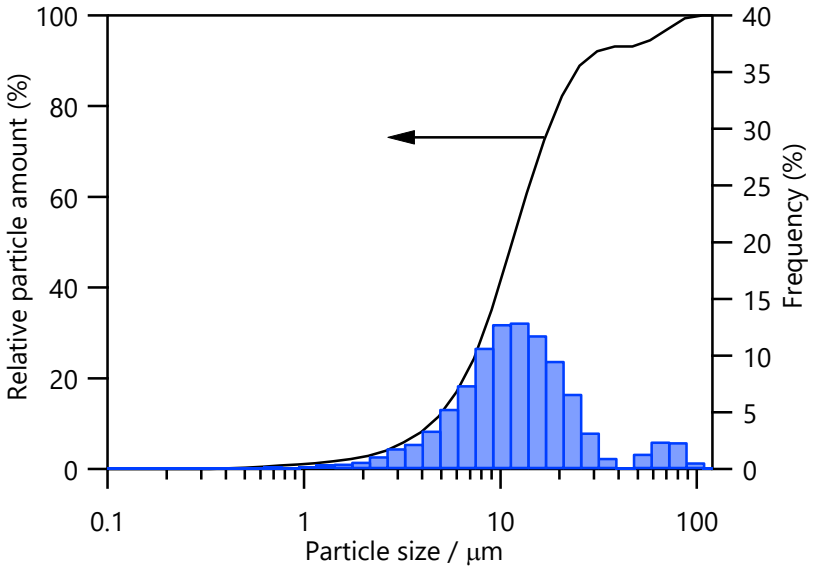


Figure S6. Dynamic light scattering (DLS) particle size distribution of $K_2Ti_2O_5$ nanosheet colloidal solution.

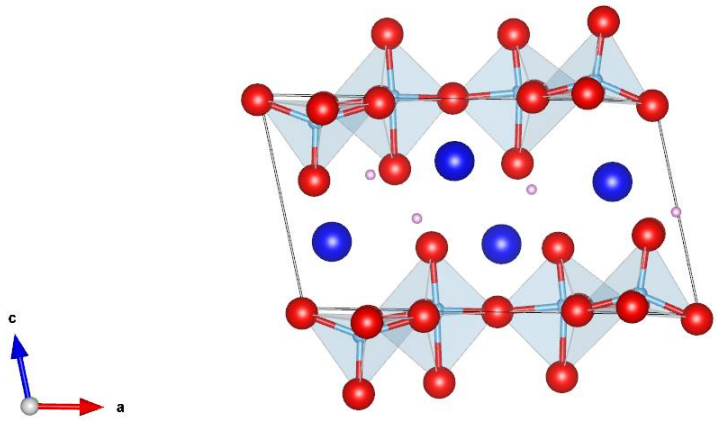


Figure S7. Calculated crystal structure of $K_2Ti_2O_5$-H_2O formed through the hydrolysis of $K_2Ti_2O_5$: a = 1.1840821 nm, b = 0.3855605 nm, and c = 0.6552678 nm, α = 85.06169°, β = 102.60363°, and γ = 89.79617°. Blue, light blue, red, and pink spheres represent K, Ti, O, and H, respectively.