

Supplementary Information

On the structure of H_2TiO_3 —a short discussion on “Lithium recovery from salt lake brine by H_2TiO_3 ”

Cheng-Long Yu,*^a Fei Wang,^a Shu-Yao Cao,^a Dan-Peng Gao,^a Huai-Bing Hui,^{a, b}

Ying-Yan Guo^c and Dao-Yi Wang^a

(^a School of Materials Science and Engineering, Shaanxi University of Science & Technology, Xi'an 710021, China; ^b Technology Research Institute, Technical Center at Dongfeng Commercial Vehicle Company Limited, Wuhan 430056, China; ^c College of Resources and Environment, Shaanxi University of Science & Technology, Xi'an 710021, China)

* To whom correspondence should be addressed.

Address: School of Materials Science and Engineering, Shaanxi University of Science & Technology, Weiyang District, Xi'an City, Shaanxi Province, 710021, China;

E-mail: johnyucl@aliyun.com (Prof. C.-L. Yu);

Tel.: +86-29-86168688;

Fax: +86-29-86168688.

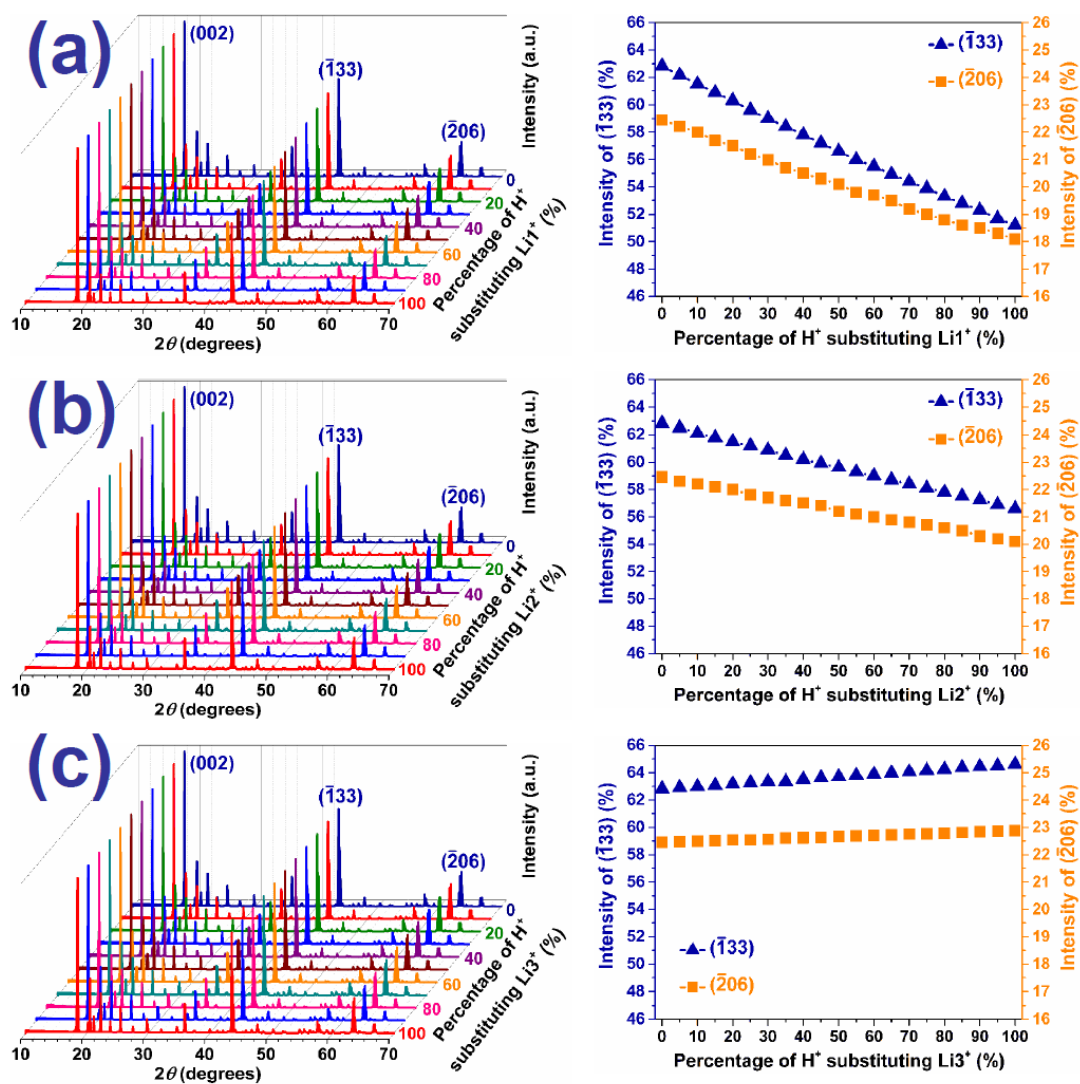


Fig. S1 Simulated XRD patterns of Li_2TiO_3 (left column) and the relative intensity variation of peak $(\bar{1}33)$ and peak $(\bar{2}06)$ by substitution of Li^+ with H^+ (right column): (a) H^+ substituting $\text{Li}1^+$ from 0% to 100%; (b) H^+ substituting $\text{Li}2^+$ from 0% to 100%; (c) H^+ substituting $\text{Li}3^+$ from 0% to 100%.

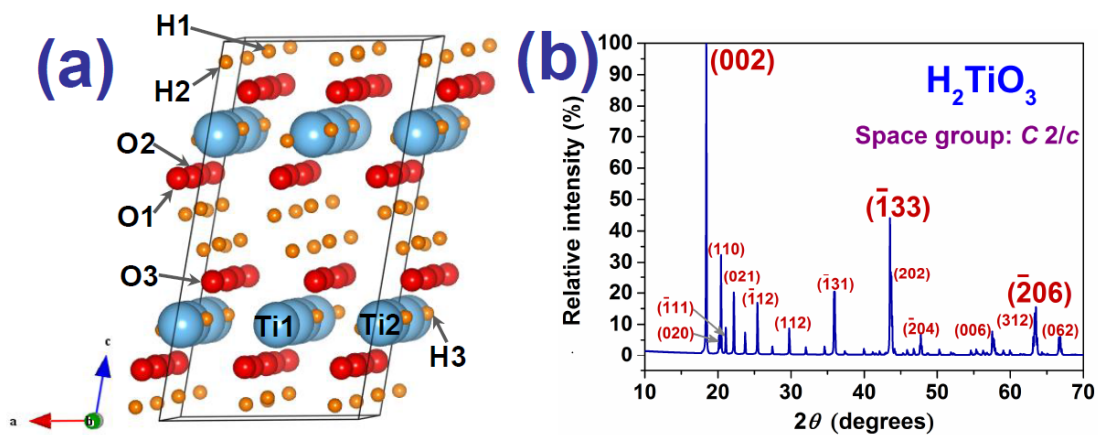


Fig. S2 The structure of H_2TiO_3 with reasonable OH bond length (a), the small orange, large blue and medium red balls correspond to H, Ti, and O atoms; and the simulated XRD pattern (b). Note that the intensity of peak $(\bar{1}33)$ and that of peak $(\bar{2}06)$ decrease by 19 % and 7 % compared with that of Li_2TiO_3 , respectively.

Table S1. Atomic coordinates and equivalent isotropic displacement parameters (\AA^2) for H_2TiO_3 .

Atom	x	y	z	U_{eq}
H1	0.13958	0.90588	0.03568	0.0147(10)
H2	0	0.26356	0.4434	0.0161(15)
H3	0.10555	0.58444	0.23604	0.0040(8)
Ti1	0	0.41749	0.25	0.00581(6)
Ti2	0	0.74971(6)	0.25	0.00575(7)
O1	0.14116(15)	0.26356(12)	0.13720(7)	0.0054(2)
O2	0.10555(14)	0.58444(16)	0.13719(7)	0.00549(18)
O3	0.13958(15)	0.90588(14)	0.13454(7)	0.0056(2)