

## **Preparation of hexagonal prism anatase with highly thermally stability from HTiOF<sub>3</sub> precursor**

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Table S1. The XRD analysis and theoretical calculation of HTiOF<sub>3</sub><sup>26</sup>.

$d_{\text{exp}}$ [Å]	$2\theta_{\text{exp}}$ [°]	$d_{\text{cal}}$ [Å]	$2\theta_{\text{cal}}$ [°]	h	k	l
14.020	6.312	14.055	6.296	0	0	2
23.741	3.745	23.691	3.752	1	0	0
27.602	3.229	27.652	3.223	1	0	2
28.081	3.175	28.328	3.148	0	0	4
34.142	2.6249	33.753	2.653	1	1	0
37.043	2.425	37.253	2.412	1	0	4
42.638	2.119	43.067	2.099	0	0	6
43.764	2.067	44.627	2.029	1	1	4
48.401	1.879	48.479	1.876	2	0	0
49.503	1.840	49.738	1.832	1	0	6
50.620	1.802	50.732	1.798	2	0	2
54.799	1.674	54.647	1.678	1	2	0
55.617	1.651	55.806	1.646	1	1	6
56.859	1.618	56.724	1.622	2	1	2
57.800	1.594	57.103	6.612	0	2	4
59.362	1.556	58.601	1.574	0	0	8
63.024	1.474	62.687	1.481	1	2	4
66.366	1.407	66.831	1.399	2	0	6
68.825	1.363	69.364	1.354	1	1	8
70.758	1.330	70.987	1.327	2	2	0
71.641	1.316	71.991	1.310	1	2	6
76.301	1.2470	76.025	1.2508	3	0	0
77.441	1.2314	77.786	1.2268	0	3	2
78.600	1.2161	78.110	1.2226	2	2	4

26. P. Liu, Y. Wang, H. Zhang, T. An, H. Yang, Z. Tang, W. Cai and H. Zhao, *small*, 2012, 8, 3664-3667.