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# A new synthetic method of titanium oxyfluoride and its application as an anode material for rechargeable lithium batteries



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## HIGHLIGHTS

- TiO<sub>2</sub> is reacted with hydrofluoric acid to produce TiOF<sub>2</sub> with a cubic perovskite structure.
- The TiOF<sub>2</sub> delivers a high charge capacity 526 mAh g<sup>-1</sup> with retention above 94% from second cycle.
- TiOF<sub>2</sub> adopts Li<sup>+</sup> ions into the cubic perovskite structure to form LiTiOF<sub>2</sub>.
- LiTiOF<sub>2</sub> phase separates to LiF and TiO by further lithiation.
- The converted TiO is converted to TiO<sub>2</sub> repeatedly in amorphous state upon cycling.

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## ABSTRACT

This paper introduces a novel, efficient method for the synthesis of TiOF<sub>2</sub>, and outlines the mechanisms of TiOF<sub>2</sub> on discharge (reduction) and charge (oxidation). Anatase TiO<sub>2</sub> is reacted with hydrofluoric acid, HF, to produce TiOF<sub>2</sub>. The synthesized TiOF<sub>2</sub> is crystallized into a cubic perovskite structure with a *Pm3m* space group, as confirmed by Rietveld refinement of X-ray diffraction data. The particles show peculiar cubic-shaped secondary particle morphology. Electrochemical investigation indicated that the TiOF<sub>2</sub> delivers a high charge capacity 526 mAh g<sup>-1</sup>. X-ray diffraction, X-ray photoelectron spectroscopy, X-ray absorption spectroscopy, and transmission electron microscopy are employed to elucidate the reaction process. During lithiation, TiOF<sub>2</sub> adopts Li<sup>+</sup> ions into the cubic perovskite structure to form LiTiOF<sub>2</sub>, and the phase separates to LiF and TiO by further lithiation. The formed TiO is oxidized to TiO<sub>2</sub> during charging although those oxides are in an amorphous state. The electrochemical reaction seems to be fairly stable, retaining 94.5% of its capacity during 100 cycles, starting from the second cycle. Also, the electrode is suitable for operation at high rates, namely, 400 mAh g<sup>-1</sup> at 200 mA g<sup>-1</sup>, 345 mAh g<sup>-1</sup> at 1.6 A g<sup>-1</sup>, and 288 mAh g<sup>-1</sup> at 3.2 A g<sup>-1</sup>.

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## 1. Introduction

Recent advances in the development of portable electronic devices such as SMART phones and tablets PCs require higher capacity rechargeable batteries to extend operation time. Sustainability of those power sources is an important factor to ensure durability of

the applications. So far, carbon-based materials are preferred for the anode (negative electrode) material because of their moderate capacity (372 mAh g<sup>-1</sup> theoretically) and good reversibility. The capacity must be increased to satisfy the requirement of a high energy battery.

There are three main categories of anode materials: intercalation/deintercalation, alloy/de-alloy, and conversion reactions. Intercalation chemistry, graphite [1,2], soft [3] and hard carbons [4,5], TiO<sub>2</sub> [6–10], and Li<sub>4</sub>Ti<sub>5</sub>O<sub>12</sub> [11–15] are considered to be the best choices because of their reasonable long-term capacity. Alloy formation reactions such as Si and Sn are being considered for

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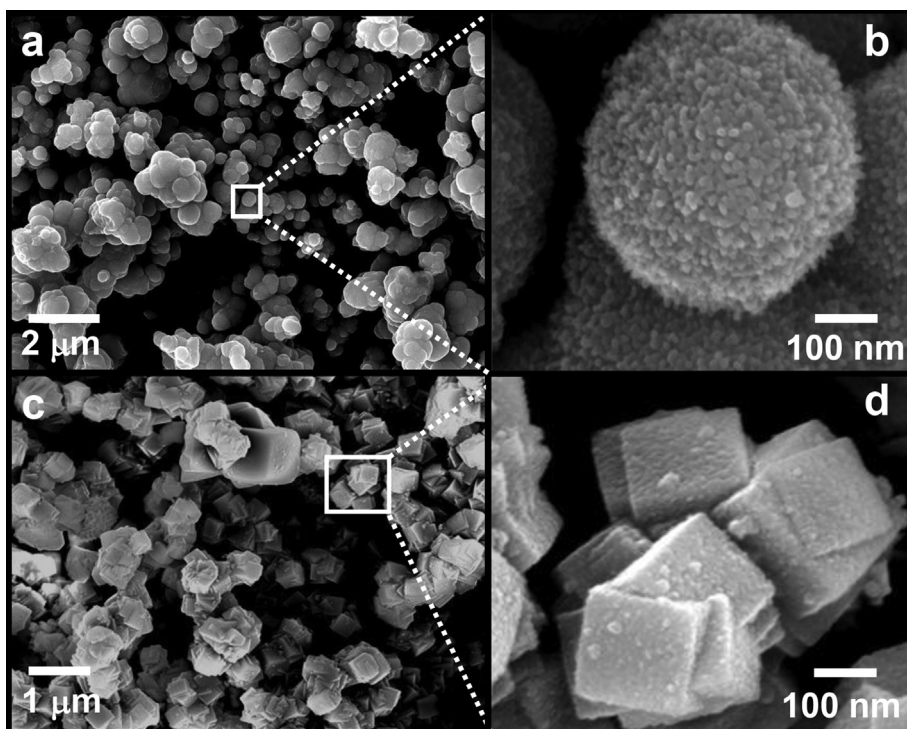


Fig. 1. SEM images: (a) hydrothermally synthesized anatase TiO<sub>2</sub> and (b) its magnified image; (c) as-synthesized TiOF<sub>2</sub> and (d) its magnified image.

future battery improvements because the alloying–dealloying process gives rise to large capacities [16–18]. However, the volume expansion of those materials (Li<sub>x</sub>Sn and Li<sub>x</sub>Si) during the alloying reaction does not retain the reversible capacity of the materials due to disintegration of electrode geometry. New research has focused

on improving the capacity retention of Si- and Sn-based alloy materials by varying binders [19,20] or forming composites with carbon [21–23] to minimize the resulting volume change. In conversion chemistry, crystalline metal oxides are reduced to amorphous metals, releasing oxygen from the parent structure [24–28].

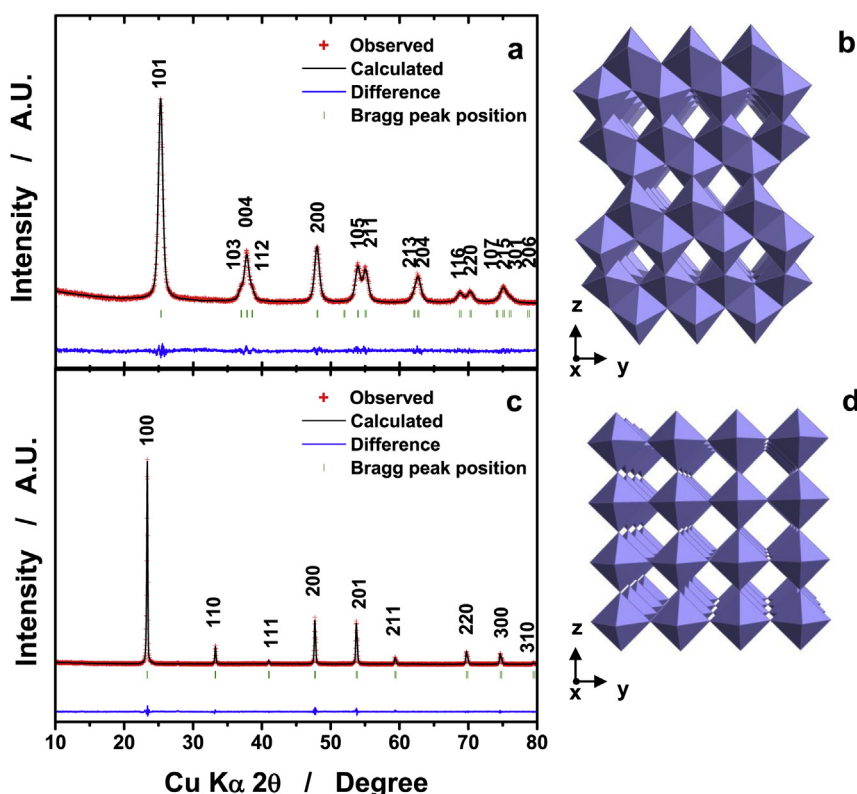


Fig. 2. Rietveld refinement results of XRD data: (a) as-synthesized anatase TiO<sub>2</sub> and its (b) structural scheme; (c) as-synthesized TiOF<sub>2</sub> and (d) the resulting crystal scheme.

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