

Supporting Information

Catalyst-free Synthesis, Structural and Mechanical Characterization of Single Crystalline $\text{Ca}_2\text{B}_2\text{O}_5\cdot\text{H}_2\text{O}$ Nanobelts and Stacking Faulted $\text{Ca}_2\text{B}_2\text{O}_5$ Nanogrooves

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Experimental

The chemical compositions and oxidation states of the $\text{Ca}_2\text{B}_2\text{O}_5\cdot\text{H}_2\text{O}$ (CBOH) nanobelts and $\text{Ca}_2\text{B}_2\text{O}_5$ (CBO) nanogrooves were further characterized by X-ray photoelectron spectroscopy (XPS) (a Kratos Axis Ultra DLD instrument equipped with a monochromated Al K_α X-ray source and a hemispherical analyzer with an energy resolution of 0.5 eV) and Fourier transform infrared (FTIR) spectroscopy (a Perkin Elmer Spectrum 100 FTIR spectrometer with a Diamond ATR attachment).

Supplemental Figures

Supplemental Figure 1

XPS spectra of the CBOH nanobelts and CBO nanogrooves, labeled as α and β , respectively. Calibration was carried out by taking the binding energy of the C 1s core level at 284.8 eV. Both survey spectra, shown in Figure 1a, exhibit Ca 2p (346.2 eV), Ca 2s (437.6 eV), B 1s (188.2 eV), O 1s (532 eV) and C 1s (284.8 eV) core levels, and no other impurity levels were detected, further indicating the high purity of the

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products. In Figure 1b, the peaks at 346.2 eV and 349.8 eV can be assigned to Ca $2p_{3/2}$ and Ca $2p_{1/2}$, respectively. Figure 1c shows the B 1s XPS spectra, the peak at 188.3 eV can be attributed to B $1s_{1/2}$ core level. As shown in Figure 1d, there are two peaks (530.0 eV and 531.7 eV) for O 1s state in the CBOH nanobelts. This is probably due to two different oxidation states of O 1s at the molecule CBOH, one of which is for the CBO molecule, and another is for the hydrated H_2O molecule.

Supplemental Figure 2

FTIR spectra of the CBOH nanobelts and CBO nanogrooves. For the CBOH nanobelts (Figure 2a), the adsorption band at 3353 cm^{-1} can be assigned to the stretching mode of O-H.¹⁻² There is no adsorption band detected at $1600\text{-}1700\text{ cm}^{-1}$, which arises from the bending mode of H-O-H, and this result indicates that the compound doesn't contain crystal water.³ The adsorption bands at 1414, 1321 and 911 cm^{-1} result from the asymmetric and symmetric stretching modes of $B_{(3)}\text{-O}$, respectively. The band at 1155 cm^{-1} is related to the in-plane bending mode of B-O-H. The weak band at 875 cm^{-1} comes from the symmetric stretching mode of $B_{(4)}\text{-O}$.³ The very strong band at 708 cm^{-1} originates from the out-of-plane bending mode of $B_{(3)}\text{-O}$.^{1,3} As for the CBO nanogrooves (Figure 2b), there is no adsorption detected at $3000\text{-}3600\text{ cm}^{-1}$, which suggests that the H_2O in CBOH has been completely removed after annealing. All other adsorption bands close to that of CBOH nanobelts have the same origins according to the previous literature.¹

References

(1) Kessler, G. Z. *Allg. Chem.* **1966**, *343*, 25-38.

(2) Liu, Z. H.; Zuo, C. F.; Li, S. Y. *Thermochim. Acta* **2004**, 424, 59-62.

(3) Li, J.; Xia, S. P.; Gao, S. Y. *Spectrochim. Acta* **1995**, 51A, 519-532.

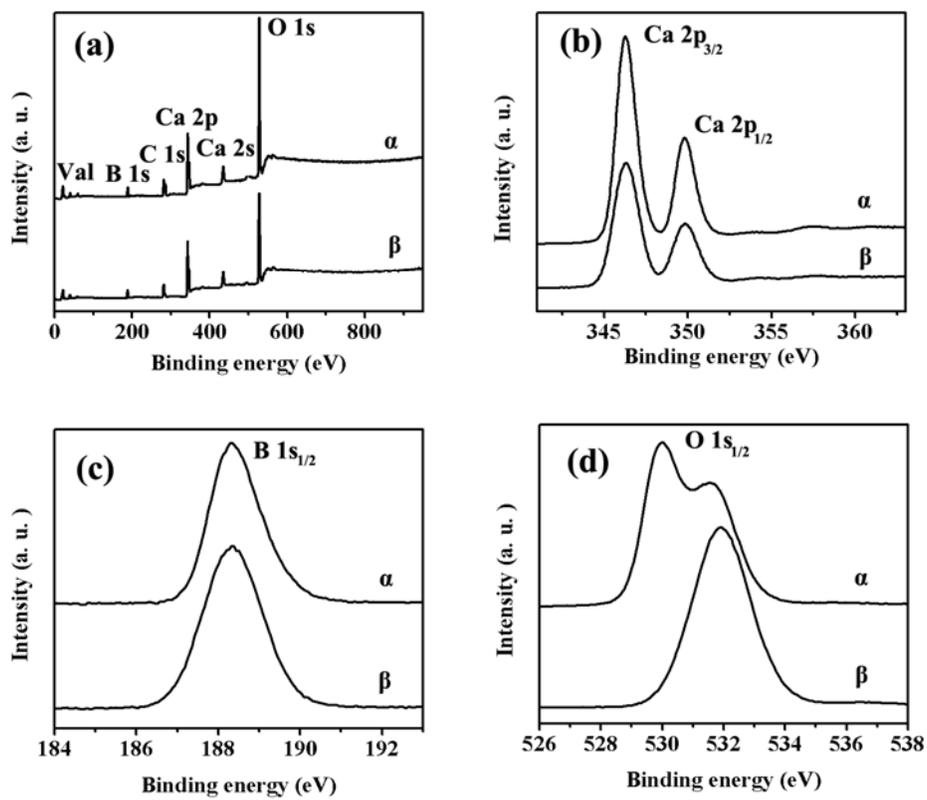


Figure 1

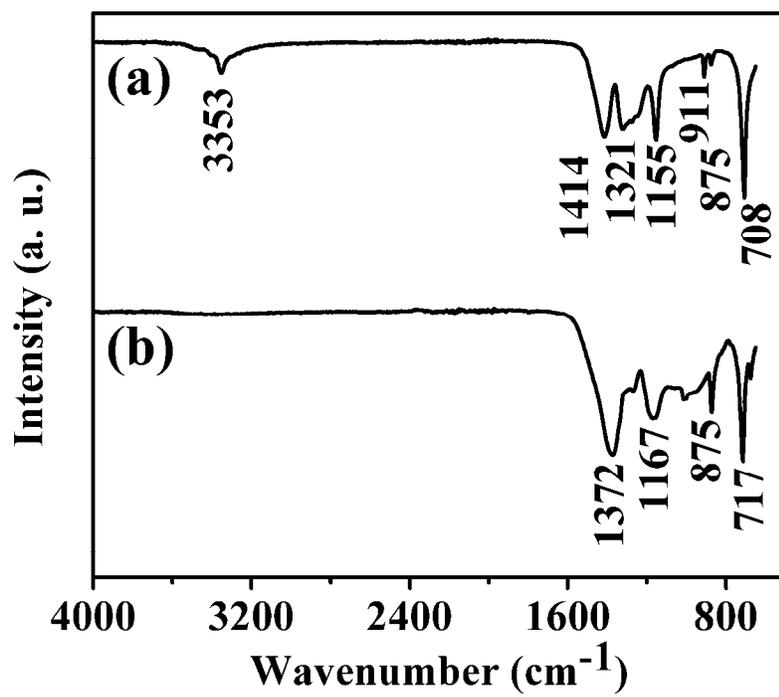


Figure 2