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Photocatalytic CO<sub>2</sub> reduction by Cr-substituted Ba<sub>2</sub>(In<sub>2-x</sub>Cr<sub>x</sub>)O<sub>5</sub>·(H<sub>2</sub>O)<sub>δ</sub> (0.04 ≤ x ≤ 0.60)

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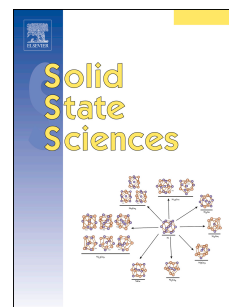
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## Photocatalytic CO<sub>2</sub> Reduction by Cr-substituted

### **Ba<sub>2</sub>(In<sub>2-x</sub>Cr<sub>x</sub>)O<sub>5</sub>·(H<sub>2</sub>O)<sub>δ</sub> (0.04 ≤ x ≤ 0.60)**

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#### Abstract

Cr-substituted polycrystalline Ba<sub>2</sub>(In<sub>2-x</sub>Cr<sub>x</sub>)O<sub>5</sub>·(H<sub>2</sub>O)<sub>δ</sub> powders (0.04 ≤ x ≤ 0.60) were synthesized by solid state reaction to investigate the relation of crystal structure, thermochemical, magnetic, and optical properties. The Cr-substitution results in an unit cell expansion and formation of the higher-symmetric tetragonal phase together with increased oxygen and hydrogen contents. Magnetic property measurements reveal that the diamagnetic pristine Ba<sub>2</sub>In<sub>2</sub>O<sub>5</sub>·(H<sub>2</sub>O)<sub>δ</sub> becomes magnetically ordered upon Cr-substitution. By UV–vis spectroscopy a gradual shift of the absorption-edge energy to lower values was observed. Numerical calculations showed that the observed bandgap narrowing was ascribed to the Cr induced states near the Fermi level. The correlation between the changes of crystal chemistry, magnetic, and optical properties of Cr-substituted Ba<sub>2</sub>(In<sub>2-x</sub>Cr<sub>x</sub>)O<sub>5</sub>·(H<sub>2</sub>O)<sub>δ</sub> can be explained by the replacement of In by Cr. Consequently, an enhanced photocatalytic CO<sub>2</sub> reduction activity was observed with increasing Cr substitution, compatible with the state-of-the-art high surface area TiO<sub>2</sub> photocatalyst (P-25).

**Keywords:** Photocatalytic CO<sub>2</sub> reduction, Ba<sub>2</sub>In<sub>2</sub>O<sub>5</sub>, DFT, Cr-substitution, Le Bail fit, crystal chemistry, magnetic property, optical property

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