

Structural and electronic modification of KLaTiO₄ hydrogen evolution catalyst

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KLaTiO₄ is a n=1 Ruddlesden-Popper type layered perovskite. KLaTiO₄ can be used as a Hydrogen Evolution Catalyst (HEC), producing 9.540 mol of H₂ gas per hour from 20 mg of catalyst, when using methanol as sacrificial electron donor and platinum co-catalyst. The main disadvantage of KLaTiO₄ is its high bandgap of 4.09 eV, above the visible light region, and therefore a poor choice for a HEC that attempts to use solar energy. To reduce the bandgap of sample to 3.10 eV (400 nm) both cationic and anionic doping of the sample is attempted. The crystal structures, and sample purity, was determined using X-ray powder diffraction. The structures have been refined by the Rietveld method using synchrotron and lab X-ray diffraction data. Hydrogen evolution was tested by illuminating a suspension of powder sample in water. Evolved gases were identified and quantified using gas chromatography.

Cationic doping of KLaTiO₄ was done by replacing lanthanum with praseodymium and ytterbium, yielding two solid solution series: KLaxPr1-xTiO₄ and KLaxYb1-xTiO₄ (x = 0.005, 0.01 and 0.03). While none of the samples from KLaxPr1-xTiO₄ series produced hydrogen, all KLaxYb1-xTiO₄ were able to produce H₂ when illuminated by a Hg lamp with 305 nm filter. In comparison to KLaTiO₄, ytterbium doped samples have a reduced catalytic activity compared to the undoped sample, as well as decrease in activity between 20 –40 minutes, before increasing in rate of production again after 40 –minute mark.

Anionic doping of KLaTiO₄ was attempted by nitrogenation, by mixing KLaTiO₄ urea and under N₂ flow. PXRD pattern of initial samples shows loss in crystallinity of KLaTiO₄ after the annealing process. Further attempts are underway, using PXRD to probe degree of sample degradation, in what is the optimal annealing condition that will achieve nitrogen doping without sacrificing complete loss in crystallinity.

Level of Expertise

Student

Do you wish to take part in the poster slam

No

Travel Funding

Yes

Speakers Gender

Male

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