Contribution ID : **18** Type : **Oral**

Structural and electronic modification of KLaTiO4 hydrogen evolution catalyst

Monday, 2 December 2019 11:35 (15)

KLaTiO4 is a n=1 Ruddlesden-Popper type layered perovskite. KLaTiO4 can be used as a Hydrogen Evolution Catalyst (HEC), producing 9.540 μmol 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.

Speakers Gender

Male

Travel Funding

Yes

Level of Expertise

Student

Do yo wish to take part in the poster slam

No

Primary author(s) : LI, Junwei (the University of Sydney, school of Chemistry)

Co-author(s) : KENNEDY, Brendan (The University of Sydney); LING, Chris (University of Sydney); Prof. MASCHMEYER, Thomas (The University of Sydney)

Presenter(s) : LI, Junwei (the University of Sydney, school of Chemistry)

Session Classification : Session 3

Track Classification : Chemistry and crystallography