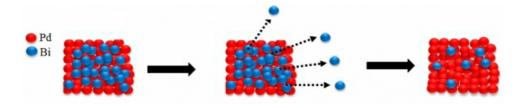
## Structural evolution in PdBi<sub>2</sub> with enhanced activity towards hydrogen evolution

<u>Shreya Sarkar</u><sup>1</sup>, Udumula Subbareddy<sup>1</sup>, Sebastian C. Peter<sup>1</sup> <sup>1</sup>Ncu, Jncasr, Bengaluru, India E-mail: sarkarshreya61191@gmail.com

Development of non-Pt based electrocatalysts for hydrogen evolution reaction is a pre-requisite for generating hydrogen, a feasible and cost-effective source of hydrogen. Structural transitions and generating metal deficiency are the effective ways of manipulating the d-band centre of a metal surface which enhances the catalytic activity of metal nanoparticles towards hydrogen evolution reaction (HER). Charge-transfer from in-situ generated oxide species to the metal centre also leads to enhancement in catalytic activity towards HER. In the present work, we report a facile colloidal synthesis of PdBi2 nanoparticles using sodium borohydride as the reducing agent. Upon annealing the as synthesized nanoparticles, a phase transition from lower symmetry monoclinic phase to higher symmetry tetragonal phase has been observed and hence, a change in morphology from agglomerated to core-shell nanoparticles. Potential cycling of both monoclinic and tetragonal PdBi2 leads to the formation of Pd-rich PdBi2-x alloy with enhanced catalytic activity (onset potential : ~19.7 mV and 29.5 mV20 mAcm-2 current density at ~140mV and ~207 mV and for monoclinic and tetragonal phases respectively). Low coordination number of Pd active sites formed by dissolution of Bi alters the d-band centre and hence, the optimal energy required for hydrogen adsorption leading to enhanced activity. Though the obtained composition after potential cycling is almost similar for the both the phases it is seen that monoclinic phase shows higher activity as compared to the tetragonal phase. Cyclic voltammetry of the monoclinic PdBi2 shows the formation of Bi-O species after potential cycling. Electron transfer from the Bi-O species to the Pd centre enhances the charge-transfer kinetics of the HER and hence an increased catalytic activity of the monoclinic phase as compared to the tetragonal phase. Hence, in-situ generated oxide species facilitates charge-transfer in-turn enhancing catalytic activity.

[1]. Jana, R. et al. (2016). ChemSusChem, 9, 2922-2927

[2]. Lv, H. et al. (2015). J. Am. Chem. Soc., 137, 5859-5862



Keywords: phase transition, dealloying, hydrogen evolution