

Title: Transition metal phosphide nanostructures encapsulated in N- & P- co-doped carbon nanotubes for water splitting in wide pH range

Abstract: In order to make clean and sustainable energy conversion, systems primarily require the development of highly efficient and robust catalysts. One of the main challenges for designing the catalysts is to minimize the cost coupled with maximum performance. Till date, noble metal-based nano catalysts had shown outstanding performances towards Oxygen Evolution Reaction (OER) and Hydrogen Evolution Reaction (HER). However, their cost and availability limits their use. Recently, phosphide nanoparticles encapsulated N & P co-doped carbon nanotubes emerge as a burgeoning class of promising electrocatalysts. This kind of structures having higher exposed active site area coupled with low cost promotes their usage compared to noble metals. In this thesis, I have described one-pot synthesis of the phosphide nanostructures which does not involve sophisticated instrumentation and cumbersome procedure and superior in terms of its activity. When the nanostructures are applied as anode for OER in 1 (M) KOH a current density of 10 mA/cm² is achieved at an overpotential of 291 mV which is less than the state of the art OER catalyst RuO₂ with a small Tafel slope of 43 mV/dec. The nanostructures also show excellent activity in 0.5(M) H₂SO₄ with overpotential of 360 mV to achieve 10 mA/cm² with small Tafel slope of 78 mV/dec. While applied as a cathode towards HER, the nanostructures exhibit a current density of 10 mA/cm² at a small overpotential of 60 mV with a Tafel slope of 66 mV/dec in alkaline medium which even outperforms the state of-the-art Pt/C catalyst. Alongside, the HER activity is quite substantial showing overpotential of 55 mV to reach 10 mA/cm² and Tafel slope of 56 mV/dec in acidic medium. After continuous electrolysis for both HER and OER, the electrode material maintains its structure along with its robust catalytic activity which brings out to their excellent stability and durability.