Designing smart materials for efficient energy conversion: The story of transition metal chalcogenides

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Energy harvesting from solar and water has created ripples in materials energy research for the last several decades, complemented by the rise of Hydrogen as a clean fuel. Among these, water electrolysis leading to generation of oxygen and hydrogen, has been one of the most promising routes towards sustainable alternative energy generation and storage, with applications ranging from metal-air batteries, fuel cells, to solar-to-fuel energy conversion systems. In fact, solar water splitting is one of the most promising method to produce Hydrogen without depleting fossil-fuel based natural resources. However, the efficiency and practical feasibility of water electrolysis is limited by the anodic oxygen evolution reaction (OER), which is a kinetically sluggish, electron-intensive uphill reaction. A slow OER process also slows the other halfcell reaction, i.e. the hydrogen evolution reaction (HER) at the cathode. Hence, designing efficient catalysts for OER process from earth-abundant resources has been one of the primary concerns for advancing solar water splitting. In the Nath group we have focused on transition metal chalcogenides as efficient OER electrocatalysts. We have proposed the idea that these chalcogenides, specifically, selenides and tellurides will show much better OER catalytic activity due to increasing covalency around the catalytically active transition metal site, compared to the oxides caused by decreasing electronegativity of the anion, which in turn leads to variation of chemical potential around the transition metal center, [e.g. lowering the Ni^{2+} --> Ni^{3+} oxidation potential in Ni-based catalysts where Ni^{3+} is the actually catalytically active species]. Based on such hypothesis, we have synthesized a plethora of transition metal selenides including those based on Ni, Ni-Fe, Co, and Ni-Co, which show high catalytic efficiency characterized by low onset potential and overpotential at 10 mA/cm^2 [Ni_3Se_2 - 200 - 290 mV; Co_7Se_8 - 260 mV; $FeNi_2Se_4$-NrGO - 170 mV (NrGO - N-doped reduced graphene oxide); $NiFe_2Se_4$ - 210 mV; $CoNi_2Se_4$ - 190 mV; Ni_3Te_2 – 180 mV].