

Renewable Energy and Energy Storage Room Naupaka Salon 4 - Session RE1-TuM

Electrochemistry and Photocatalysis II

Moderator: Craig Perkins, National Renewable Energy Laboratory

9:00am RE1-TuM-4 Tuning Optoelectronic Properties of 2D Transition Metal Dichalcogenides and p-Conjugated Polymers, *Elisa Miller*, National Renewable Energy Laboratory **INVITED**

This talk will review recent research tuning optoelectronic properties of 2D transition metal dichalcogenides (TMDCs) and p-conjugated polymers to ultimately control energy conversion processes. First, a major roadblock to the commercial deployment of TMDC monolayers for next generation electronic devices has been the inability to controllably dope these materials at wafer scale as can be done with traditional semiconductors. We demonstrate dedoping with high spatial fidelity in wafer-scale monolayer MoS₂ upon illumination with a mechanistic understanding. Second, the p-conjugated polymer n-type N2200 and P90 polymers (alternating naphthalene dicarboximide (NDI) acceptor and bithiophene (T2) donor units, where NDI units in P90 alternately feature methyl end-capped heptaethylene glycol (90%) and 2-octyl dodecyl (10%) side chains) are studied to understand how electrolyte cation insertion influences the polymer electronic behavior, which is necessary for energy conversion applications.

9:40am RE1-TuM-6 Transition Metal Doped NiOx Faceted Nanosheets for Electrocatalytic Water Oxidation, *Konstantin Ruecker*, German Aerospace Center Oldenburg, Germany; *Dereje Taffa*, Carl von Ossietzky University of Oldenburg, Germany; *Elliot Brim*, *Darius Hayes*, Colorado School of Mines, USA; *Julian Lorenz*, German Aerospace Center Oldenburg, Germany; *Shaun Alia*, *Bryan Pivovar*, National Renewable Energy Laboratory; *Marcel Risch*, Hemholtz Center Berlin, Germany; *Corinna Harms*, German Aerospace Center Oldenburg, Germany; *Michael Wark*, Carl von Ossietzky University of Oldenburg, Germany; *Ryan Richards*, Colorado School of Mines, USA

The ability to manipulate earth abundant metal oxides presents an important potential technology to develop sustainable materials with novel properties. These materials are of interest due to the coordination environments that can be achieved and to the high degree of control over properties that can result from tailoring the exposed facets of metal oxides. Here, recent highlights regarding nanostructured metal oxides and their applications in electrocatalysis will be presented. Water electrolysis enables the production of green hydrogen as part of the energy transition. Moving to alkaline media using an anion exchange membrane (AEM) enables the usage of non-precious metal electrocatalysts and thereby limitations in the availability and the cost of catalyst materials required for proton exchange membrane water electrolysis. The oxygen evolution reaction (OER) at the anode involves multiple electron and proton transfer steps and thus suffers from a higher overpotential than the hydrogen evolution reaction at the cathode, making catalyst development for the OER critical for water electrolysis. Transition metal oxide (TMO) catalysts are promising as efficient electrocatalysts for the OER in alkaline media, since they are relatively active and the material is comparably inexpensive. It has been shown, that the electrocatalytic activity of nickel-based catalysts is strongly influenced by the morphology, by the crystallographic orientation of the material and by the combination of different transition metals into the nickel oxide host structure.

In this study, NiO nanosheets predominantly oriented in the (111) crystallographic planes were synthesized by either hydrothermal (HT) or microwave-assisted (MW) routes, to investigate the influences of faceting as well as the enhancements by doping with transition metals (Fe, Mn, Co), where especially doping with small amounts of Fe (e.g. 5 mole %) enhanced the OER activity. Furthermore, the syntheses were adopted to produce Fe, Mn and Co doped NiO (111) nanosheets with various dopant concentrations. The Fe and Co doped NiO (111) nanosheets outperformed the pure NiOx materials during the testing, whereas the Mn doping decreased the electrocatalytic activity of the materials. Structural characterization by synchrotron-based X-ray absorption spectroscopy and X-ray photoelectron spectroscopy before and after electrochemical testing were used to elucidate underlying processes like phase transformation and oxidation state changes.

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