ADREBO - ADditives for REchargeable high-energy Bivalent metal-Organic batteries - ABSTRACT

The aim of the research project is to enhance the properties of bivalent (Mg, Ca) next generation batteries with organic cathodes. The main issue of the contemporary multivalent batteries is electrolyte speciation, which leads to ion pair formation and poor multivalent ion desolvation. On the anode side ion pair formation leads to decreased anion reductive stability leading to poor metal plating/stripping efficiency and formation of blocking passive layer. On the cathode side single charged ion pair can act as charge carriers changing electrochemical mechanism from high-energy battery based on multivalent cation exchange to low-energy dual ion battery due to high amount of electrolyte salt needed for full cathode capacity utilization.

In our proposal we will prevent ion pair formation and promote multivalent ion desolvation in Mg and Ca electrolytes by use of electrolyte additives. In first stage commercial additives will be used to probe the effect of different functional groups. Obtained data from testing of commercial additives combined with the results of theoretical calculation will be used to guide the synthesis of tailored made additives. Main research hypothesis is built on exploring not only interactions between bivalent cations and chelating additives, but also interactions between salt anions and anion receptor – additives. We postulate that the presence of properly designed functional groups in additives structure enables partial immobilization of anions and improve salt dissociation, further leading to synergies between the cation and anion targeting additives. Modified electrolyte solutions will be applied to newly developed nanostructurized organic cathode materials based on benzoquinone electroactive group.

Specific objectives of research project are:

- **Determination of best cation and anion additives for ion pair dissociation and multivalent cation desolvation in multivalent electrolytes by screening research with use of DFT & MD calculations**
- **Preparation of best cation and anion additives for ion-pair dissociation and multivalent cation desolvation in multivalent electrolytes**
- **Finding the synergies between the best performing cation and anion additives**
- **Preparation of high-energy n-type organic polymer high energy with practical capacity over 300 mAh/g**
- **Achieving metal plating/stripping efficiency above 99% in multivalent electrolytes**

Realization of these objectives will allow us to move beyond current state-of-the-art on the multivalent batteries and create basic body of knowledge necessary for realization of the high-energy density multivalent metal–organic batteries. To achieve these ambitious goals, we join two experienced PIs with an extensive track record on the development of multivalent batteries (Dominko, NIC) and development of both electrolytes and their additives (Wieczorek, WUT). On the longer time scale development of high-energy density multivalent metal batteries could boost competitiveness of Polish, Slovenian industry and wider EU industry, which does not have a good access to raw materials used in contemporary Li-ion batteries and has listed them as critical.

A cutting-edge nature of this project will be enabled by highly specialized know-how of both partners in the consortia. Group at NIC specializes in the studies of multivalent batteries and application of organic cathodes, while group at WUT has extensive experience with use of additives and modification of electrolytes. Thus, we were already able to identify key bottlenecks in the field of multivalent battery research, performance of multivalent electrolytes, and have devised sensible research approach to quickly move beyond current state-of-the-art with expertise of group at WUT.