Polyimides as organic cathode materials for magnesium batteries

Mg batteries are promising post-Li battery technology due to their improved safety, volumetric capacity, price and abundance. It has been shown that traditional inorganic intercalation cathodes are not the best fit for multivalent Mg ions, while organic cathode materials seem as favorable option on account of their flexible, open structure.

This thesis is about studying polyimides as cathode materials in Mg batteries. Not much data is published about polyimides as cathodes in Mg system and our goal was to explore their general Mg electrochemistry. Initially we focused on exploring various synthetic conditions and observed how it affected the electrochemical performance in a battery. Electrochemistry in Li system served us as an early indicator how a certain polymer behaves as a cathode. Besides having a better cycling performance in terms of stability, Li-organic system is more understood. The next step was synthesis and battery cycling of some novel polymers, which were not yet published at that point.

In the last part of the thesis, our focus was building better understanding of electrochemical mechanism of charge storage in Mg system. We briefly compared polyimide Mg electrochemistry to quinones to see if they share similar mechanism. More detailed study of charge storage mechanism was performed by *in-operando* infrared spectroscopy, which was supported by density functional theory study.

Because of polyimides insolubility, we were notably limited by possible analytical techniques. We used elemental analysis, infrared spectroscopy, solid-state nuclear magnetic resonance and scanning electron microscopy. Some effort was devoted to determination of possible impurities within polymer chains.

Polyimides were found to be electrochemically active in Mg system, with confirmed electrochemical mechanism of carbonyl bond reduction. Mg electrochemistry is even more complex than Li and we could not thoroughly estimate role of polyimides as a cathode since there seem to be many factors, that are tightly intertwined and co-dependent, especially electrolyte and its fine balance of electroactive species.