DESCRIPTION FOR THE GENERAL PUBLIC

The main objective of this research project is the investigation of the electrochemical processes of intercalation of lithium and sodium ions in to the structure of electrode materials based on REM_2 and RE_5M_3 (where RE=rare-earth metals, M=Sn, Pb and Sb), which can be used as anode materials for lithium- or sodium-ion batteries which have a higher electrochemical activity, higher energy density, improved kinetics of electrode processes, higher chemical stability, less harmful to the environment and a lower cost of production, as compared to currently used Li_xC anode material.

Li-containg intermetallic compounds from large metal atoms, which crystallize in structures with sufficiently large octahedral voids to insert lithium on vacant interstitials without severe structural changes are hardly investigated. This project will elucidate the preconditions for Li-insertion in selected REM_2 and RE_5M_3 model systems with $ZrSi_2$ and Mn_5Si_3-type structures and their structural response. These compounds are expected to form sufficiently large tetragonal antiprism and also octahedral voids for RE=rare-earth metals, especially Sm and Gd, and M=Sn, Pb or Sb to allow a reversible Li-insertion. A comprehensive structural investigation will compile the relevant aspects for the filling of tetragonal antiprism and octahedral voids with lithium and details of the type of bonding. The aim of this project is to establish a new class of Li-containing ternary intermetallic compounds derived by the reversible filling of tetragonal antiprismatic and octahedral interstitials with better cyclic stability.