Subproject JP3.1

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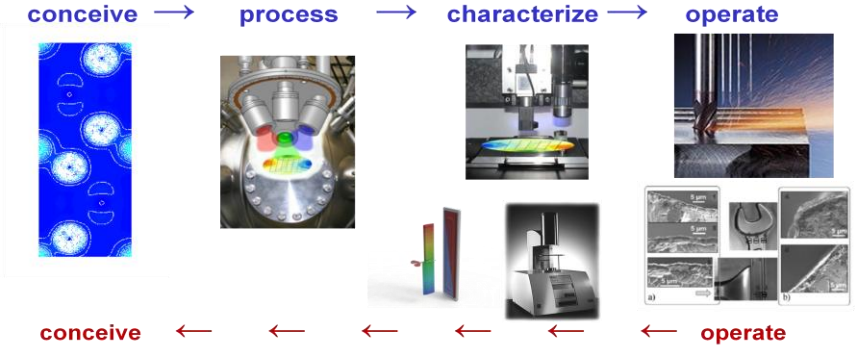
Project description

Based on the quantum mechanically guided design proposal for anodes, we will synthesize combinatorial thin films of the ternary compounds exhibiting a large Li mobility and a low volume expansion. Density and bonding analysis of a selected MA–Al–Si amorphous alloy will be used to verify the calculated *ab initio* data. Also, cell voltages of the proposed anodes will be estimated using *ab initio* calculations. Our partners at KIT will determine the cell voltages and ionic conductivity of Li in these MA–Al–Si thin films upon exposure to molten Li. These theoretical and experimental efforts will not only provide composition proposals for future anodes with enhanced performance but will also shed light on the composition induced changes in electronic structure that govern the diffusivity and volume expansion.



The equipment used to prepare amorphous MA–Al–Si thin films is a UHV sputtering chamber. The sputtering unit has four separate cathodes which are arranged at an angle to each other and to the substrate. This setup can produce concentration gradients in the film along the substrate surface and this strategy is also known as a composition spread or a combinatorial approach. Based on the quantum mechanically guided design proposal, we will synthesize combinatorial thin films of the ternary compounds exhibiting a large Li mobility and a low volume expansion. We will systematically investigate the process parameter window for combinatorial magnetron sputtering of amorphous MA–Al–Si thin films (MA = selected from *ab initio* MD). The main process parameters varied here are the power density at the MA, Si and Al magnetron targets and the Ar total pressure. We will adjust the magnetron power densities of the individual sources so as to obtain the desired compositions. We will obtain the synthesis-chemical composition correlations for these amorphous anodes. This will be verified at KIT and compared with the *ab initio* data.

Another *ab initio* calculation task to be carried out at MCh is the selection of MC in the cathode system Li–Mn–O–MC (MC = Co, Ni, Ti, Al, Si). The density functional theory at 0 K, as described above, we be used. We will calculate energies of formation for major competitive phases, such as orthorhombic and spinel. These data will be used at KIT as input for phase diagram modelling and selection of the MC element in Li–Mn–O cathode system.