# Continuum Modeling as a Tool for Battery Development – Form material to cell scale

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Batteries are essential to our daily lives. Majority electrical devices are powered by state-of-the-art lithium-ion batteries. However, the number of applications, and therefore the demand and requirements for batteries, are constantly growing. In particular, the electrification of the mobility sector, from battery electric vehicles to electric aircrafts, poses significant challenges for future battery technologies. Key performance indicators are energy density, safety, sustainability and cost. For new battery technologies to meet the requirements of a specific application, novel materials, electrode and cell designs need to be developed.
In this talk, I will give an overview of our work on the continuum modeling of batteries - from state-of-the-art lithium-ion technology to new cell chemistries including sodium-ion, metal-sulfur and solid-state batteries.
Virtual Material Design is a method developed by DLR and its partners that combines versatile and efficient tools for material development. In our previous work, it has been used extensively for the design of electrode architectures for Li-ion batteries [1]. In addition, the tools allow to account for heterogeneities and defects introduced providing a link to the manufacturing process [2,3].
Similar tools with a similar level of complexity and predictive power have yet to be developed for new battery technologies [4,5]. Extensions to the models and tools are needed to capture the specific features of the various new cell chemistries. Examples that will be addressed in this contribution are hierarchically structured porous active materials for sodium-ion batteries, the formation and dissolution of solid charge and discharge products in Li-S batteries, or the effect of grain boundaries on the design of solid-state batteries.
The goal of our work is to develop the simulation tools to couple the relevant scales for material and cell design and to provide guidelines for the development of current and next generation batteries.

References:
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