

# The importance of passive materials in thick Li-ion battery electrodes

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Due to their outstanding energy and power density, Li-ion batteries are widely used. The porous composite of a Li-ion battery electrode generally consists of active material, conductive carbon and polymeric binder. The so-called carbon binder domain (CBD) is distributed in the macro-pores of the electrode and both, provides better mechanical stability as well as electronic contact. However, at the same time the CBD increases the tortuosity of Li-ion transport pathways in the electrolyte. At high current densities, this increases mass transport limitations and reduces the performance of the battery cell<sup>1</sup>. It has already been shown that the production process has a significant effect on the morphology and spatial distribution of the CBD.

In our contribution we present results of pore scale simulations in Li-ion batteries<sup>2</sup>, which explicitly consider the morphology and spatial distribution of the CBD. In these simulations we study 3D realizations of NMC cathodes created by a 3D stochastic microstructure generator<sup>3</sup> with varying density, particle size, thickness and CBD content.

In a first step we determine effective conductivities of the virtual samples which provides insight on limiting processes during operation of the battery cell. In a second step, we simulate the electrochemical performance of the virtual electrodes with an extended version of the “Battery and Electrochemistry Simulation Tool” (BEST) considering both the transport of electrons in the conductive carbon network as well as Li-ion transport in the pore space of the CBD. In our simulations we see that insufficient contact and high electronic resistance reduces the capacity at low CBD content. Interestingly electronic conductivity is not limiting the electrode capacity at high electrode densities, which opens up new strategies for the electrode design of for high-energy density batteries.

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## References:

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