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Theory and Modelling of Novel Materials for High Energy Batteries

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Summary

Energy storage is particular important for advanced fuel-efficient vehicles and mobile applications, rechargeable batteries play a key role for such applications. Lithium-ion batteries are today the leading energy storage systems. However, the cathode materials remain insufficient for the use of lithium-ion batteries. To improve this drawback, cathode materials has to be developed further. Therefore, today, most research is focused on the cathode material, and a precise knowledge of the diffusion/transport behaviour of lithium cations inside battery-cathode materials is critical for improving energy density, material properties, and for estimating the impact of chemical substitution. Computer simulations down to an atomistic scale mainly based on density-functional theory (DFT) have been proven to be a strong tool for achieving a fundamental understanding of their properties as well as to search for completely novel materials.

We will report especially results of DFT based calculations on known (e.g. LiMPO4, M=Ni, Fe, Mnol) and new cathode materials(e.g. Borate based materials), their stability and their structural and electronic properties. Additionally, results of simulations of Li transport properties within selected cathode materials will be shown. We point out that capacity and diffusion/conduction issues must be understood in a much more detail-rich framework, under realistic simulation conditions within finite temperature simulations. Along this line we unravel a diverse set of diffusion pathways, without the need to artificially speed-up Li diffusion by large temperatures.