

Today, more than ever, rechargeable batteries are silent companions in our day-to-day lives serving as energy storage units in all sorts of devices. Overall battery performance is a result of many factors. The combination of development choices made during material selection, cell design, pack design and charging strategy will impact the battery performance in the final use phase. The complexity of optimization problem spreads over a number of steps in the value chain, i.e. starting materials, materials' composition, synthesis conditions, slurry preparation, coating and drying, calendaring, cell assembly, choose of electrolyte and formation.

The massive migration from fossil fuels to electric enforces the availability of capable batteries. Thus, this proposal on novel design of Li-Ni-Mn-Co (NMC) cathode materials for high energy batteries is in agreement with a long-term research initiative of EU Battery2030+, where the goal is to demonstrate 5-10-fold improvement in materials discovery. However, considering materials like NMC one should take into account that in long-term perspective lots of those complex materials have to be recycled, so the elemental composition of the future batteries should be as simple as possible, allowing the efficient recycling and recovery of critical materials in terms of economic importance or risk supply.

The main goal of the proposal is to find a forward-looking design of only NMC system leading to a new class of electrochemical materials for Lithium-ion batteries (LIBs). This two-dimensional structure imparts high Li^+ mobility to the material. Despite the extensive studies, a single optimal composition has not been found yet for the NMC since each of constituent cations has a different role to play in the cathode material. There is a demand to compromise high electrochemical capacity and cycle retention, safety and environmental beingness.