

Lithium-ion batteries (LIBs) have become a key technology in the move towards a greener and more sustainable future. These energy storage solutions have revolutionised various industries, including electric vehicles, renewable energy systems and portable electronics. The growing demand for cleaner energy sources, coupled with the European Green Deal and the United Nations' commitment to limit temperature increases to 1.5 degrees Celsius, has contributed to the rapid growth of the lithium-ion battery market. Researchers and manufacturers are striving to make cells more efficient, cheaper and safer.

One of the priorities of recent research has been to reduce cobalt content, due to its toxicity, price and ethical concerns about its extraction. Nickel-based materials are very popular due to their high capacity. However, their cyclic and thermal instability is an issue that needs to be addressed. Therefore, an understanding of the changes occurring during the charge and discharge cycles of the cells is sought. This is a very complex process and requires in-depth study by multiple methods. One method to help unravel this problem is Raman spectroscopy. Using this technique in situ (during cell operation) can show structural changes such as phase transitions and structure degradation occurring during intercalation and deintercalation of lithium ions in the material structure. However, in order to fully analyse the resulting spectrum, information on the position of the individual peaks present in the spectrum is needed.

The main objective of this project is to analyse the position of the peaks corresponding to the individual bonds in lithiated manganese-cobalt nickel oxide (NMC). This problem has so far also been addressed by calculations using quantum mechanics methods, but the results obtained so far are subject to large error. The proposed solution will allow the analysis of Raman spectra to be simplified and more information to be extracted from studies carried out in this way. To achieve this, materials with different nickel/manganese ratios will be used and the position of individual peaks will be determined from changes in the appearance of the spectra. The approach to solving this problem is innovative and obtaining the information sought will be a revolution in the field.