PhD position:
Simulation of heterogeneities in battery cells with low environmental impact materials

Supervisors: Benoît MATHIEU, Luc LECOINTRE, Marion CHANDESRIS
Location, dates: CEA Grenoble, three year PhD position with flexible starting date near 09/2025
This position is internally funded by CEA.

Profile : We are looking for someone with a strong interest in multi-physics phenomena and a degree in either applied Mathematics, Physics, or Engineering. More specific knowledge on python, finite-volume/finite elements methods, high-performance computing, the physics of transport phenomena would also be greatly appreciated.

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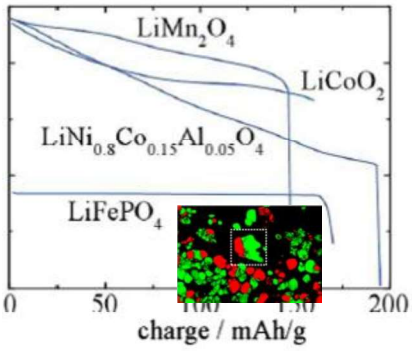
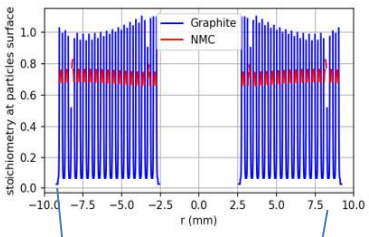
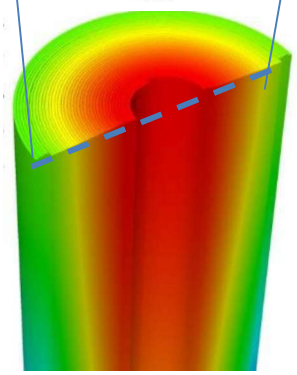
The electrification of vehicles to decarbonize our activities faces a dilemma concerning batteries, their environmental impact and the supply of materials needed to manufacture them. The low-environmental-impact materials being considered today to meet these needs (LF(M)P, sodium-ion technology, etc.) have specific electrochemical characteristics that need to be anticipated before they can be used in large-capacity batteries. These two- or multi-phase materials have an electrical potential that is only slightly dependent on the state of charge. This characteristic favours the appearance of a highly heterogeneous state of charge in the cell. The complex mechanism is linked in particular to fast charging, which is very important for vehicles, and which creates significant heating at the heart of the cells. These heterogeneities limit battery performance and shorten their lifespan. In addition, the flat voltage profile and heterogeneities make it extremely difficult to diagnose the cell's state of charge and state of health. Yet this information is crucial for battery management that maximizes battery life.
Our laboratory is developing advanced modeling tools that enable us to simulate these phenomena. Using a highly detailed numerical model of a large cell, applied to realistic cycling conditions, the candidate will highlight the internal state of cells, which is difficult to access experimentally, and show how cycling, thermal management or diagnostic strategies need to be adapted for the more sustainable chemistries envisaged today. To do this, he will use CEA's software platforms and supercomputers, and draw on CEA/LITEN's expertise covering all technological stages, from materials to real-life cell testing.







Fine 3D multiphysics model of a cylindrical cell.
Top figure: example of potential profiles for various active materials with/without 2-phase behaviour.
Middle: stoichiometry profile during a fast charge though the entire roll of electrodes
bottom: temperature field