To launch a COMSOL simulation:

- 1. Open Template.mph (COMSOL 5.6)
- 2. Click on "Browse" in the Mesh/"Import" tab and select your mesh file (.bdf)
- 3. Don't click on "import" but click on "All Domains" in the Definitions/"Selections" tab
- 4. Once the mesh has been imported, tick "All domains" in Definitions/Selections/"All Domains" tab
- 5. Click on Definitions/Selections/"CBD", then click on "Add" ("+" sign) and add "ID 3 Import 1"
- 6. Click on Definitions/Selections/"Separator", then click on "Add" ("+" sign) and add "ID 21 Import 1"
- 7. Click on Definitions/Selections/"NMC811", then click on "Add" ("+" sign) and add all the items starting from "ID 1001 Import 1" to the bottom
- 8. Click on Definitions/"Current Collector", then click on "Geometry", then "Measure"



- 9. Click on Definitions/"NMC811", then click on "Geometry", then "Measure"
- 10. Click on Global Definitions/"Parameters", then copy paste the surface (displayed in the "Messages" tab) of the current collector into the "Surface_CC_Solid" variable, and the volume of the NMC into the "VolumeNMC" variable
- 11. Press "compute"

Notes:

- If you are using an electrode with a different thickness, you have to modify in Definitions/Selections/"Box Li Foil" the parameter "z minimum" accordingly. Here z minimum = 156 μm (150 μm electrode + 6 μm separator).
- 2. If you want to simulate a discharge at a different C-rate you have to modify the "C_rate" parameter in Global Definitions/Parameters. For instance, C_rate = 0.5 = C/2. Also, in Study/Step2: Time-Dependent, in "Output times", modify accordingly the timestep at which the solution will be saved. The format is the following (starting time, timestep,end time).
- 3. If you encounter a "self-intersecting face" error when importing a mesh, right-click on "Mesh 1", select Intersections and Partitions/"Detect Faces", add the ID of the faces self-intersecting based on the error message, and put Maximum_neighbor_angle = 20°