

*Simulation files can be used using Matlab 2017a. The data set contains the following folders and files*

- **extrapolating\_Ubat**: extrapolating towards zero current to determine  $U_{bat}$ , see Section 4.1 of the paper
- **figure\_making**: allows reproducing the figures of the paper
- **numerical\_illustration**: compare model output when giving a perturbation to nominal values of parameters, see Section 5.2.2. of the paper.
- **Parameters estimation\_alpha\_sep**: parameter estimation using LM method. In the file, main\_estimate.m is the main file and predict\_erro.m is the minimizing function, see Section 5.3 of the paper
- **sensitivity**: using QR factorization to do parameter ranking, see Section 5.2.1 of the paper
- **simulation\_DFN**: simulate the DFN model, Section 6 of the paper. Parts of the m-files are re-used from "Lu J. Development of fast one-dimensional model for prediction of coupled electrochemical/thermal behavior of Lithium-ion batteries. Bachelor's thesis, The Ohio State University; 2013." The model produces the following outputs
  - Cs: solid concentration
  - Ce: electrolyte concentration
  - Phie: electrolyte potential
  - Phis: solid potential
  - Cse: surface concentration in solid phase
  - cell\_voltage: terminal voltage