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DEM-based modelling of the mechanical and electrical behavior of lithium-ion battery electrodes

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Bearing in mind the particulate nature of lithium-ion battery electrodes, this work proposes a discrete element method (DEM) simulation approach to describe such porous composite structures. To this purpose, a Hertzian-bond contact model was developed in order to capture the elasto-plastic behavior of the electrode by computing bonds between particles under certain conditions and combining, thus, both particle and binder stiffness. This simulation tool provides an essential comprehensive understanding of how the interaction among all components may affect the structural and mechanical properties of lithium-ion battery electrodes.

Once assured that the structure as well as the mechanics could be appropriately captured by this DEM simulation approach, the goal was set on the prediction of the conductivity. In order to fulfill this task, the A* computer algorithm was implemented in Python and run complementary to the DEM simulation. This algorithm is well known in computer science for its performance and accuracy and is widely used in pathfinding and graph search. This whole methodology helps assist in predicting the electrical conductivity that can be used in larger scale continuum models. A full comprehensive study was carried out to give insight into the influence of electrode porosity and thickness, particle size distribution and composition of the electrode. Considering that finding optimal electrode design which balances competing trade-offs can be challenging [1,2], such a valuable tool can help understand the influence of electrode structure and mechanics on battery performance.

Finally, it was aimed to study the evolution of the electrical conductivity under mechanical loading. The objective was to derive a relationship between the structural and mechanical behaviour of the electrode and its conductivity when external pressure is applied. This correlation is not only relevant for the performance of the battery but also for safety aspects.

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