A computational journey from the electronic structure to the mesoscale... and back!

The emerging properties of complex materials result from processes and interactions taking place at different scales in hierarchical order. Multi-scale simulations take advantage of capturing the relevant phenomena at a given scale, relying on good approximations to decrease the level of description of a system, thus increasing the size and complexity of the sample investigated. In this talk, I will demonstrate a computational protocol using first-principle calculations to model atomic and coarse-grained force fields in a bottom-up fashion. I will present mesoscale simulations using the MOLC model, a coarse-grained (CG) force field initially developed to describe organic semiconductors. Unlike most CG models, MOLC reproduces the excluded volume of molecules at a level comparable to atomic force fields. This unique characteristic allows the reverse-mapping of atomic coordinates, which are suitable for electronic structure calculations. Multi-scale simulations based on the MOLC model will be discussed, along with the potential application for the study of battery performance optimisation.