Machine learning for predictive modelling of energy nanomaterials

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Project outline

Nanoparticle (NP)-based functional heterogeneous materials are promising candidates for applications in energy harvesting and storage devices/systems (e.g. Li-ion batteries). Multiple internal interfaces present in those materials (e.g. as boundaries between NPs and surrounding matrix materials) play an important role in structural integrity and overall long-term performance of energy-related systems. Hence, truly *predictive modelling* of those materials must account for atomistic properties and features of their interfaces to provide a new insight into performance enhancement and optimisation of nanomaterials for energy applications.

This project *aims* at developing a predictive *machine-learning* (*ML*) approach to account for *atomistic uncertainty* in interfacial behaviour, and its subsequent propagation onto the microscopic (material morphology) and macroscopic (device/system) length and time scales. In particular, a *Bayesian inference* approach will be developed, numerically implemented (Matlab/Python) and used to predict interfacial material laws governing interface strength from available non-equilibrium atomistic simulation data.

Case studies will include predictive modelling of the mechanical response of interfaces between active graphene nanoparticles and the surrounding effective matrix material (cf. Fig. 1a). Those material systems show nanoscopic damage when subject to in-service conditions (cf. Fig. 1b), which leads to a noisy interfacial response at the atomistic level (cf. Fig. 1c).

The project can be extended into developing *ML* approaches to capture more realistic coupled response (e.g. electro-chemo-mechanical) of energy materials and their interfaces.

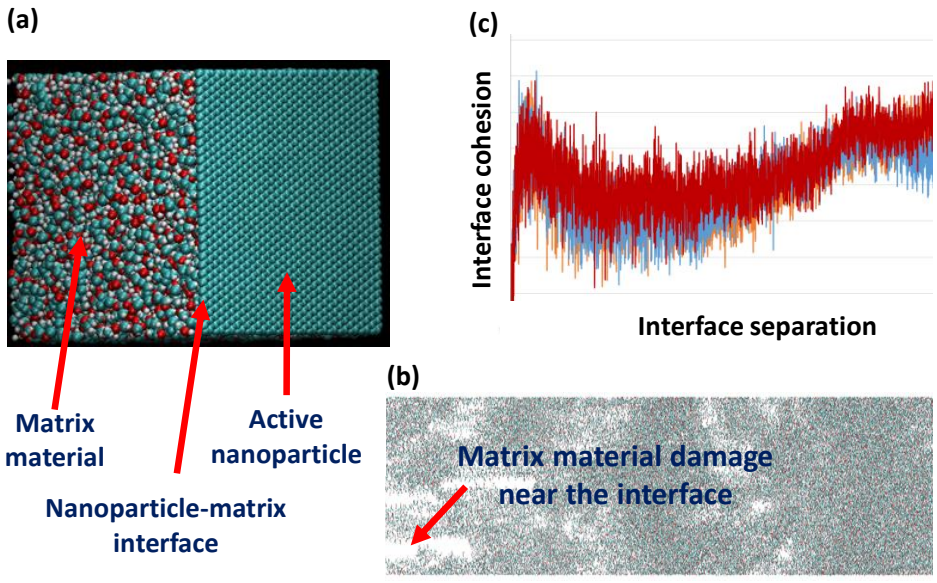

Fig. 1: *Interfacial failure in a nanoparticle-based heterogeneous material for battery electrodes; (a) atomistic model of the interface; (b) non-equilibrium atomistic prediction of nanoscopic damage; (c) atomistic predictions of cohesion force – interface separation curves*