Modelling gaps (and benefits) at the electronic and atomistic levels in industry

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Key Words: *DFT, interatomic potentials, battery cathodes, fuel cells, industry*

Being a leading speciality chemical company in the sustainable technologies, Jonson Matthey was an early adopter of atomic scale modelling techniques. The use of computational modelling has grown in the company and DFT and interatomic potential methods are now routinely used in a diverse portfolio of internal projects, ranging from cars' catalytic converters to high energy density Li-ion battery materials. This impulse presentation will focus on our modelling research efforts in the automotive electrification area. I will show how screening several potential dopants using atomistic modelling techniques allowed us to improve the battery performances of our $LiFePO_4$ cathode materials. A selection of dopants is shown to impact charging performance and the cyclability of the cathode materials.
However, despite its successes, some pitfalls remain where DFT methods face difficulty in giving a satisfactory answer. The talk will review the challenges faced in modelling battery materials. Li-ion cathode are particularly difficult to accurately model because they are composed of transition metal oxide with strong electron correlation. In addition, their structure is highly complex with varying oxidation states, dynamic Li migration and the presence of interfaces. One example from our activities in fuel cell development will finally highlight how these pitfalls can manifest themselves when investigating transition metal oxides [1].

REFERENCES

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