Simulations lithium intercalation into a Li_xFePO4 battery electrode during recharging with kinetic Monte Carlo method

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The demand for reliable and high energy density batteries for use in hybrid and plug-in hybrid vehicles requires improvements of currently available lithium batteries systems. One strategy is to use fine-particle electrode materials that provide large surface area for lithium ion intercalation in electrochemical processes. Thus, the role of interfaces in the transport and reaction behaviour becomes more important for informed battery-microstructure design. These roles have been studied experimentally and by modelling . More particularly, we will show how battery modelling can account for complex and different reactions that takes place at electrode interfaces for different experimental conditions, such as charging rate.

A kinetic Monte Carlo algorithm based on rigid lattice was used to study kinetic of lithium intercalation into a Li_xFePO4 electrode during a galvanostatic discharge. This algorithm takes into account:

- the structure of both phases in presence (e.g. $Li_\alpha FePO_4$ and $Li_{(1-\beta)}FePO_4$)
- the solubility limit of Li in $FePO_4$
- the role of the Volmer-Butler relation on lithium ion interface transport
- the configuration dependent activation barriers within the lattice.

The results provide insight into the role atomistic behavior in microstructure development and phase transitions during recharging.

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