Insight into the lithiation mechanisms in Li-ion anode materials by x-ray absorption spectroscopy

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For the investigation at the atomic scale of battery materials, X-ray Absorption Spectroscopy (XAS) is largely used, as a valuable tool to monitor electronic and structural changes occurring through electrochemical cycling, with unaltered sensitivity even in case of nanocrystalline or amorphous phases that commonly form upon Li^+(or Na^+)-uptake/release.
Within this contribution we will report results of recent studies on zinc and iron oxide materials, notably carbon coated transition metal doped zinc oxide (TM-ZnO) and zinc ferrite (ZnFe2O4) nanoparticles storing lithium by a conversion and alloying mechanism.
These materials have been recently reported as a very promising alternative anode material for Li-ion batteries enabling enhanced reversible capacity exceeding 1000 mAh/g (almost three times higher than state-of-the-art active material graphite) and improved cycling stability even at high rate[1].
The further optimization of such class of materials requires full understanding of the electrochemical (de-)lithiation reaction mechanism at the atomic scale. The main focus of the XAS spectroscopic characterizations was therefore on probing oxidation state and local structure of the metal centers on pristine materials[2,3] as well as on cycled electrodes by both ex-situ and operando experiments with synchrotron radiation[4,5].

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References

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