X-ray spectroscopic studies of materials for energy applications

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We have studied Li_xFePO_4 olivine, $Li_xMn_2O_4$ spinel and Li_xCoO_2 ceramic materials, which are used as cathodes in lithium batteries. The transition metal oxidation number can be monitored with the L-edge x-ray absorption spectroscopy (XAS) [1]. In general, XAS reveals the electronic structure of unoccupied energy levels of the sample while x-ray emission spectroscopy (XES) gives the complementary information about the occupied energy levels. All these spectra can be either predicted or verified by first-principles calculations. Moreover, the theory predicts that techniques based on inelastic x-ray scattering can be used to detect the elusive lithium. In particular, x-ray Compton scattering can directly image electronic orbitals associated with lithiation as demonstrated in a recent study of $Li_xMn_2O_4$ [2]. So far, we have shown that x-ray spectra can be successfully predicted using first-principles. Thus, we have enabled a fundamental characterization of lithium battery materials involving spectroscopy and first-principles calculations. The detailed information we have obtained regarding the evolution of electronic states will be indispensable for understanding and optimizing battery materials.

References

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