Facile synthesis of nano-structure LiCoPO4@UiO-66 particles and its *in-situ* XAS, structural properties and electrochemical characterization for lithium batteries

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Nanostructured LiCoPO₄@UiO-66 were facilely synthesized by MW- assisted solvothermal in one pot-coating at three hours. We introduce a facilely and novel route to enhance the conductivity and the performance of electrochemical properties. The X-ray diffraction pattern of the as-synthesized samples was indexed to a single olivine orthorhombic structure with a Pnma space group, as shown in figure a. TEM analysis exhibited that the particle size of LiCoPO₄ was reduced due to the additive of UiO-66 into precursor solution, and there are small particles of ZrO_2 coated the LiCoPO₄ owing to post-annealing, as exhibited in figure b. The first discharge capacity of the LiCoPO₄@UiO-66 electrode was 146 mAh.g⁻¹ at 0.05 C in a voltage range of 3.0- 5.27 V, corresponding to approximately 87% of its theoretical capacity (167 mAh/g) as shown in figure d. The X-ray absorption for the as-synthesized samples confirmed the phase is a single and orthorhombic structure with space group Pnma- LiCoPO₄ in agreement with calculated spectra by FDMNES, as shown in figure c. At this point, the aim was to determine the local environment of the Co, upon the lithiation/de-lithiation process, while testing the *in-situ cell* at the C/5 current rate in the 3-5.27 V voltage range. The principal component analysis (PCA) showed that the LiCoPO₄@UiO-66 has two components implying to the noted degradation referred to the resistance of the electrolyte, as shown in figures e,f.



[1] Kozawa T, Kondo A, Fukuyama K, Naito M, Koga H, Shimo Y, et al. (2019) J Solid State Electrochem.;23(4):1297-302.

[2] Li W, Song B, Manthiram A.(2017) Chem Soc Rev 46(10):3006-59.

[3] Wolfenstine J, Read J, Allen JL.. (2007) J Power Sources;163(2):1070-3.

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