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## Structural and computational analysis of $Y_{0.88}Ni_{3-x}Mn_x$ compounds to understand the localization of Mn atoms

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Intermetallic compounds  $AB_n$  ( $A$ =rare earth, Mg;  $B$ =early transition metal,  $2 \leq n \leq 5$ ) can store large amount of hydrogen. They have been investigated as negative electrode materials for Ni-MH batteries due to their outstanding electrochemical properties, including in new protic ionic liquid (PIL) electrolyte<sup>1-3</sup>.

Within this family,  $AB_3$  compounds ( $n=3$ ) are of primary importance due to their high capacity. In this work, we investigate the influence of the Mn substitution on hydrogenation and electrochemical properties of  $Y_{0.88}Ni_{3-x}Mn_x$  ( $0 \leq x \leq 1$ ) compounds. Indeed, for the close  $A_2B_7$  family ( $n=3.5$ ), Mn substitution for Ni flattens the plateau pressure, and increases the electrochemical capacity<sup>4</sup>. Moreover,  $AB_3$  system structural study is interesting, as a sub-stoichiometry of Y is needed for obtaining single-phase  $AB_3$  compounds. To understand this, density functional theory calculations have been coupled to advanced structural characterization using synchrotron X-ray diffraction at SOLEIL/Cristal beamline and neutron diffraction at ILL/D1b beamline. Joint Rietveld refinement have been performed to determine the location of Mn atoms. The lattice parameter  $a$  keeps almost unchanged while  $c$  decreases with Mn content up to  $x=0.3$ . This anisotropic behavior is directly correlated to the site-occupation of Mn atoms.

The electrochemical capacity of these alloys as negative electrode material was tested in pyrrolidinium acetate [Pyr][Ac] and KOH electrolytes. A capacity of 275 mAh.g<sup>-1</sup> was obtained for  $x=0.44$ , higher than that obtained in KOH for this material. For all compositions, the capacity decreases drastically over cycling in KOH while is stable in [Pyr][Ac], proving the interest of coupling  $AB_3$  compounds and PILs. The correlation between structural and electrochemical properties will be discussed.

### References

- [1] T. Kohno *et al.*, *J.AlloysCompds* 311(2000)5-7
- [2] V. Charbonnier *et al.*, *J.Phys.ChemC* 119(2015)12218-12225
- [3] N. Chaabene *et al.*, *J.PowerSources* 574(2023)233176\_1-7
- [4] N. Madern *et al.*, *Energies* 13(2020)3470\_1-17

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