FeNCN as new molecular negative electrode materials for Li- and Na-ion

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We report evidence for the electrochemical activity of transition metal carbodiimides versus lithium and sodium[1]. In particular, the iron carbodiimide FeNCN can be efficiently used as a negative electrode material for alkali-metal-ion batteries (Li and Na), similarly to its oxide analogue FeO. Based on ^{57}Fe Mössbauer and infrared spectroscopy (IR) data, the electrochemical reaction mechanism can be explained by the reversible transformation of the Fe–NCN into Li/Na–NCN bonds during discharge and charge processes. These new electrode materials exhibit higher capacity compared to well-established negative electrode references such as graphite or hard carbon. Contrary to its oxide analogue, iron carbodiimide does not require heavy treatments (nanoscale tailoring, sophisticated textures, coating etc.) to obtain long cycle life with density current as high as 9 A/g for hundreds of charge/discharge cycles. Similar to the iron compound, several other transition metal carbodiimides (M_xNCN_y with M = Mn, Cr, Zn) can cycle successfully versus lithium and sodium. Their electrochemical activity and performances open the way to the design of a novel family of anode materials for both Li- and Na-ion batteries.

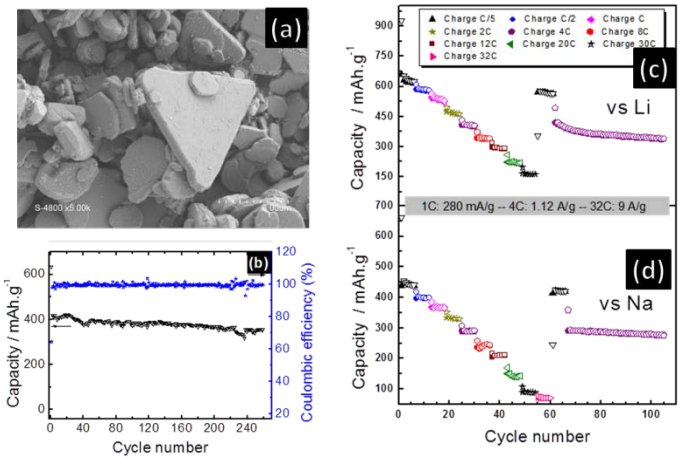

Fig. 1: SEM micrograph for FeNCN powder (a), cycle life of FeNCN/Na cell (b), capability rate vs Li (c) and Na (d)

1. Sougrati, M. T.; Darwiche, A.; Liu, X.; Mahmoud, A.; Hermann, R. P.; Jouen, S.; Monconduit, L.; Dronskowski, R.; Stievano, L., Transition-metal carbodiimides as new molecular negative elec-trode materials for Li- and Na-ion batteries with excellent cycling properties. *Angew. Chem., Int. Ed.* **2016,** Accepted.