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Electrochemical performance of CuNCN for sodium ion batteries and comparison with ZnNCN and lithium ion batteries

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HIGHLIGHTS

- Thermal stability under O_2 and N_2 atmosphere controlled by *In-situ* XRD.
- EPR spectroscopy is used to analyse reaction intermediates.
- Irreversible capacities affected by Kinetic limitations.
- Constant voltage process can increase the coulombic efficiency of the 1st cycle.
- Improved capacity retention and rate capability of CuNCN in NIBs and LIBS.

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ABSTRACT

Transition metal carbodiimides (TMNCN) undergo conversion reactions during electrochemical cycling in lithium and sodium ion batteries. Micron sized copper and zinc carbodiimide powders have been prepared as single phase as confirmed by PXRD and IR and their thermal stability has been studied in air and nitrogen atmosphere. CuNCN decomposes at ~250 °C into CuO or Cu while ZnNCN can be stable until 400 °C and 800 °C in air and nitrogen respectively. Both carbodiimides were electrochemically analysed for sodium and lithium ion batteries. The electrochemical Na^+ insertion in CuNCN exhibits a relatively high reversible capacity (300 $mAh \cdot g^{-1}$) which still indicates an incomplete conversion reaction. This incomplete reaction confirmed by ex-situ EPR analysis, is partly due to kinetic limitations as evidenced in the rate capability experiments and in the constant potential measurements. On the other hand, ZnNCN shows incomplete conversion reaction but with good capacity retention and lower hysteresis as negative electrode for sodium ion batteries. The electrochemical performance of these materials is comparable to that of other materials which operate through displacement reactions and is surprisingly better in sodium ion batteries in comparison with lithium ion batteries.