Solid State Ionic Modelling of Niobium Based Oxides for Battery Applications

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Mixed niobium based oxides are increasingly gaining research and commercial momentum as next generation battery materials. They generally present in the Wadsley-Roth (W-R) crystal structures consisting of a central block, with Nb in corner sharing sites and edge sites that adjoin neighbouring blocks. In particular, the transition of Nb (3+ → 5+) oxidation states allow for high lithium intercalation. The niobium oxides can be partnered with other transition metals (TM) such as Vanadium (V), Phosphorous (P), Tungsten (W) and Titanium (Ti) among others, to avail a plethora of materials for exploration. Ranging in the size of block (3x3 → 3x5 and mixed block systems) and varying oxidation states which result in increasing the ion storage capacity of these materials. Which makes them very attractive for battery applications.

In this keynote, several W-R materials will be discussed. Where materials modelling techniques have been used to better understand the influence of the transition metal reducibility on structural, electronic as well as transport properties. The talk will include a review of the literature as well as our most recent work, on several mixed niobium oxides. Our recent work suggests the expansion and contraction of the blocks influences the volume expansion as Li intercalates. The electronic structure calculations give insights on the reducibility of the transition metal cations while the dynamical simulations suggest favourable pathways and the influence of the TM on the transport properties.

References:

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