**Article title:** Structural transformation during Li/Na insertion and theoretical cyclic voltammetry of the δ-$NH_4V_4O_{10}$ electrode: a first-principles study

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**Abstract:** A double layer δ-$NH_4V_4O_{10}$, due to its high energy storage capacity and excellent rate capability, is a very promising cathode material for Li-ion and Na-ion batteries for large-scale renewable energy storage in transportation and smart grids. While it possesses better stability, and higher ionic and electronic conductivity than the most widely explored $V_2O_5$, the mechanisms of its cyclability are yet to be understood. Here, we present a theoretical cyclic voltammetry as a tool based on first-principles calculations, and uncover structural transformations that occur during $Li^+/Na^+$ insertion (x) into $(Li_x/Na_x)NH_4V_4O_{10}$. Structural distortions associated with single-phase and multi-phase structural changes during the insertion of $Li^+/Na^+$, identified through the analysis of voltage profile and theoretical cyclic voltammetry are in agreement with the reported experimental electrochemical measurements on δ-$NH_4V_4O_{10}$. We obtain an insight into its electronic structure with a lower band gap that is responsible for the high rate capability of $(Li_x/Na_x)$δ-$NH_4V_4O_{10}$. The scheme of theoretical cyclic voltammetry presented here will be useful for addressing issues of cyclability and energy rate in other electrode materials.