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On the origin of high performance V2O5 cathodes of aqueous Mg-ion batteries: A computational study

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Vanadium pentoxide (V2O5) is one of the promising cathode materials for Mg-ion batteries owing to its high capacity, safety, and low toxicity. However, it still suffers from sluggish charge transport kinetics and low stability. To overcome these problems, experiments reported that using aqueous electrolytes dramatically improves ion diffusion and capacity of V2O5-based cathode. Proton from water in the electrolyte may alter battery performance but its role remains unclear. Herein, we used density functional calculations to examine the effect of proton on the improved charge transfer properties and stability of Mg-proton co-intercalation to reveal the role of aqueous electrolyte. We find that protons prefer to intercalate into V2O5 and reside at vanadyl oxygen atoms. Upon proton intercalation, the band gap of V2O5 decreased from 2.17 eV to 0.07 eV suggesting better electronic conductivity. In addition, it improves Mg-ion diffusion where the diffusion barrier is reduced from 0.89 to 0.49 eV in the vicinity of intercalated proton. This work unravels the role of water in electrolyte in the enhanced cathode performance which could be used to better design cathode materials or electrolyte for Mg-ion batteries.

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