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Exploring the Surface of Vanadium Phosphate Cathode Materials

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In this study, we used a combination of synchrotron soft X-ray absorption spectroscopy (XAS), lab-scale experimental techniques and first principles computation to critically examine and validate the surface and bulk electronic structure of prototypical vanadium (III) phosphate intercalation cathode materials, Na3V2(PO4)3, Li3V2(PO4)3 and K3V3(PO4)4• H2O. Using a combination of XPS, Raman UV-Vis -NIR, UPS and DFT calculations, a full picture of each AVPs electronic structure was developed and validated using both experimental and calculated electronic structure and density of states data. From our synchrotron data, XAS fluorescence yield and electron yield measurements reveal substantial variation in surface-to-bulk atomic structure, vanadium oxidation states and density of oxygen hole states across all AVP samples. We attribute this variation to an intrinsic alkali metal surface depletion layer identified across these alkali metal vanadium (III) phosphates. We propose that an alkali-depleted surface provides a beneficial interface with the bulk structure(s) that raises the Fermi level and improves surface charge transfer kinetics at the surface of this family of materials. This surface depletion phenomenon has been previously reported in other prominent transition metal phosphate intercalation cathodes, such as LiFePO4 and its general presence here suggests wider ubiquity amongst alkali transition metal phosphate materials.

Level of Expertise

Student

Presenter Gender

Man

Pronouns

He/Him

Which facility did you use for your research

Australian Synchrotron

Students Only - Are you interested in AINSE student funding

Yes

Do you wish to take part in the Student Poster Slam

Yes

Condition of submission

Yes

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