# First-Principles Characterization of a Novel Chromium Doped Vanadyl-Oxide Based Cathode for Higher Energy and Efficiency Lithium-ion Batteries

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Lithium ion (Li-ion) batteries power almost all rechargeable devices, however, as the demand for energy storage exponentially increases, the commercially available Li-ion technology is proving to be insufficient. The primary issue with batteries lies in the cathode because of its poor energy capacity and efficiency. Recent advances in vanadium based cathodes attempt to address these problems of which, LiVOPO4 shows promising results. In this work, using LiVOPO4 as the base structure, a novel chromium (Cr) doped LiVOPO4 cathode was computationally developed using Density Functional Theory (DFT) in efforts to achieve better energy storage capabilities. The voltage regimes as a function of lithiation and the DFT energetics for various phases of Cr doped LixVOPO4 were predicted to assess its energy capacity characteristics. Furthermore, the Electron Localization Function (ELF), magnetic spin distributions, and Density of States (DOS) were analyzed to evaluate its cycling efficiency. Cr-LixVOPO4 proves to significantly increase the operating voltage regimes over the entire lithiation cycle and can intercalate extra Li past the second Li insertion (x = 2.5) at 1.2 V. The DFT relaxation of Cr-LixVOPO4 further indicates a structurally reversible framework during full delithiation and relithiation. These results suggest a fivefold increase in energy capacity compared to commercial LiCoO2 while operating at higher voltages. Cr-LixVOPO4 further maintains a high-spin state and demonstrates low electronic band gaps over the lithiation cycle, indicating a significant increase in the cycling efficiency. Overall, Cr-LiVOPO4 is predicted to have far better energy storage capabilities compared to commercial LiCoO2, making it a highly promising cathode for Li-ion batteries.

**Awards Won:**

Office of Naval Research on behalf of the United States Navy and Marine Corps: The Chief of Naval Research Scholarship Award of $15,000

Air Force Research Laboratory on behalf of the United States Air Force: First Award of $750 in each Regeneron ISEF Category