Computational and experimental materials search of potential polyanionic K-ion cathodes

Supplementary Information

Jingyang Wang[a,b+], Bin Ouyang[a,b+], Hyunchul Kim[a], Tian Yaosen[b], Gerbrand Ceder[a,b*] and Haegyeom Kim[a*]

a. Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

b. Department of Materials Science and Engineering, University of California, Berkeley, CA 94720, USA

+equal contribution

*Corresponding author:

Dr. Haegyeom Kim (Email: haegyumkim@lbl.gov)

Prof. Gerbrand Ceder (Email: gceder@berkeley.edu)

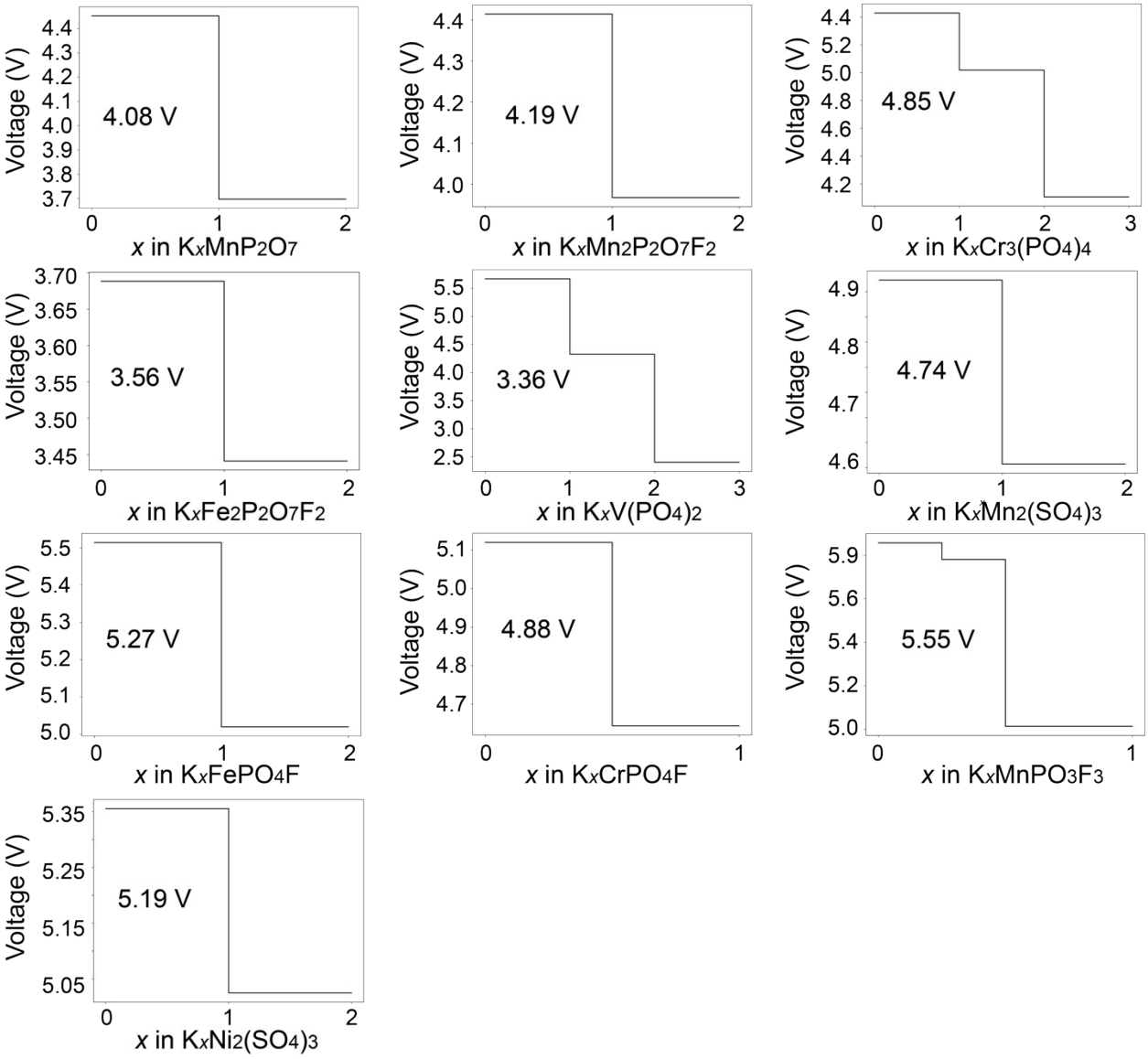

Figure S1. Calculated voltage profiles of the 10 compounds listed in Table 1.

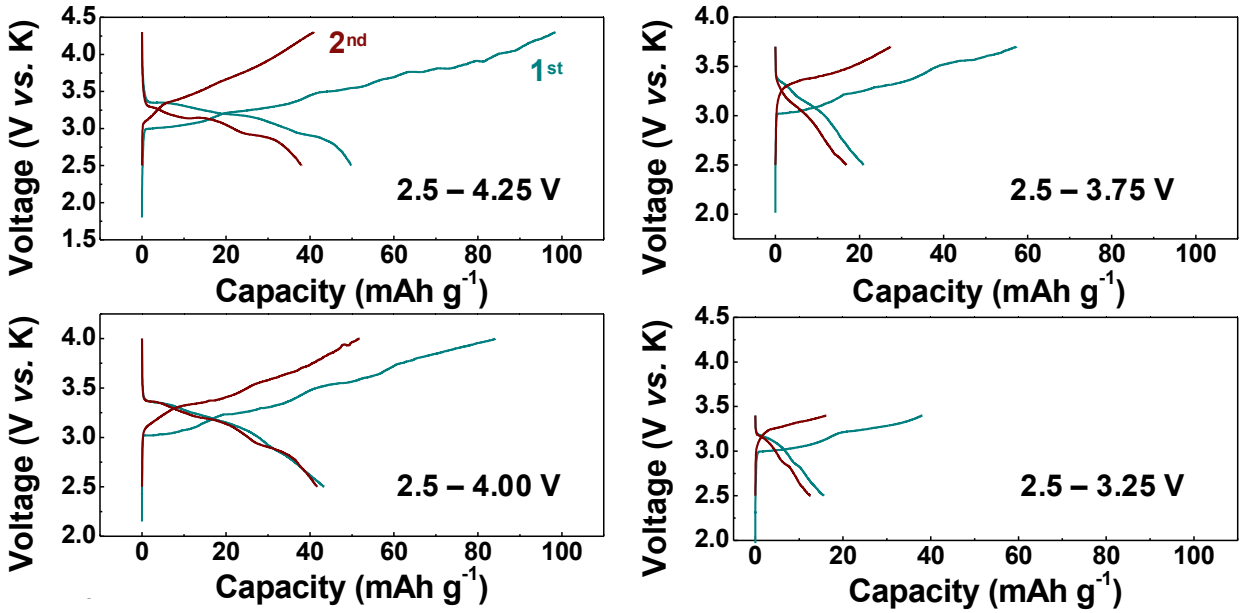

Figure S2. Electrochemical voltage profiles of $K_6V_2(PO_4)_4$ at different cut-off voltages.

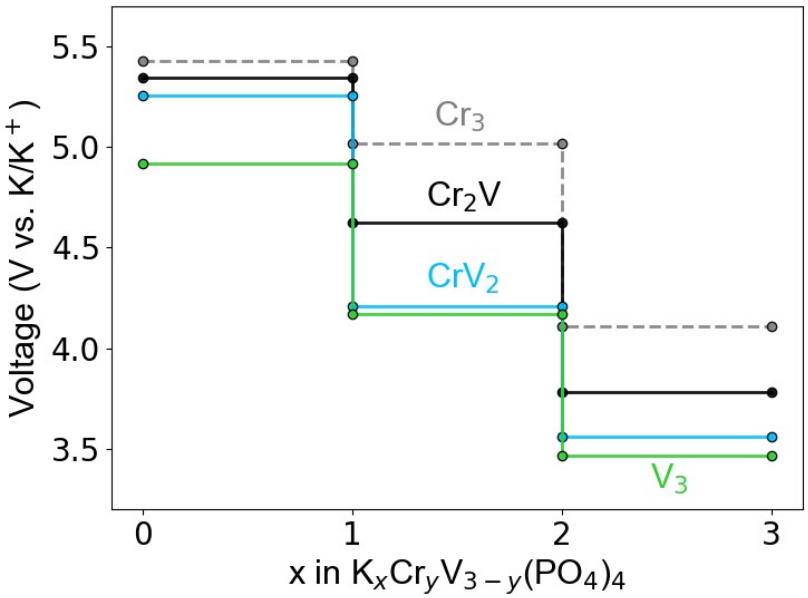

Figure S3. Calculated voltage profiles of $K_xV_{3-y}Cr_y(PO_4)_4$ (x = 0, 1, 2, 3) system.

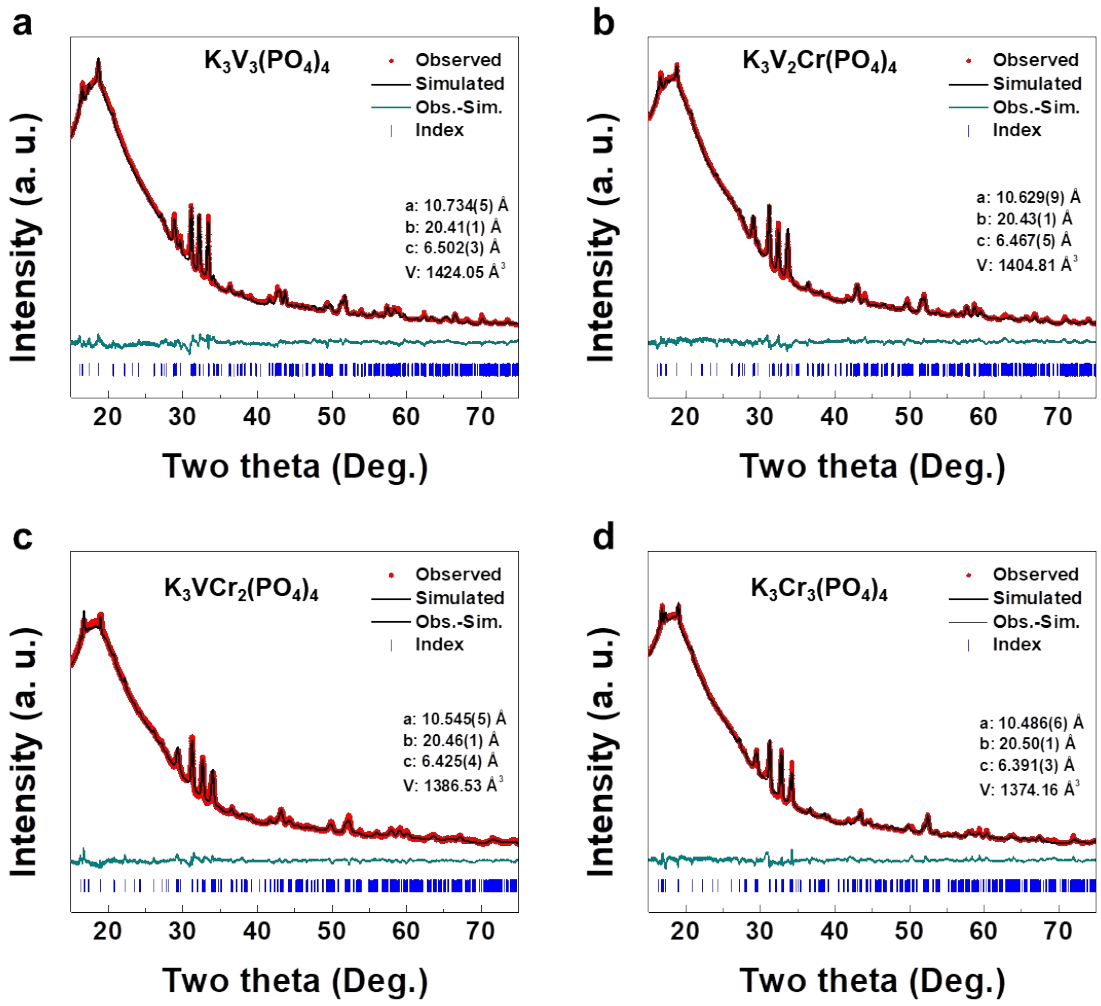

Figure S4. Refinement results of **a.** $K_3V_3(PO_4)_4$, **b.** $K_3V_2Cr(PO_4)_4$, **c.** $K_3VCr_2(PO_4)_4$, and **d.** $K_3Cr_3(PO_4)_4$.

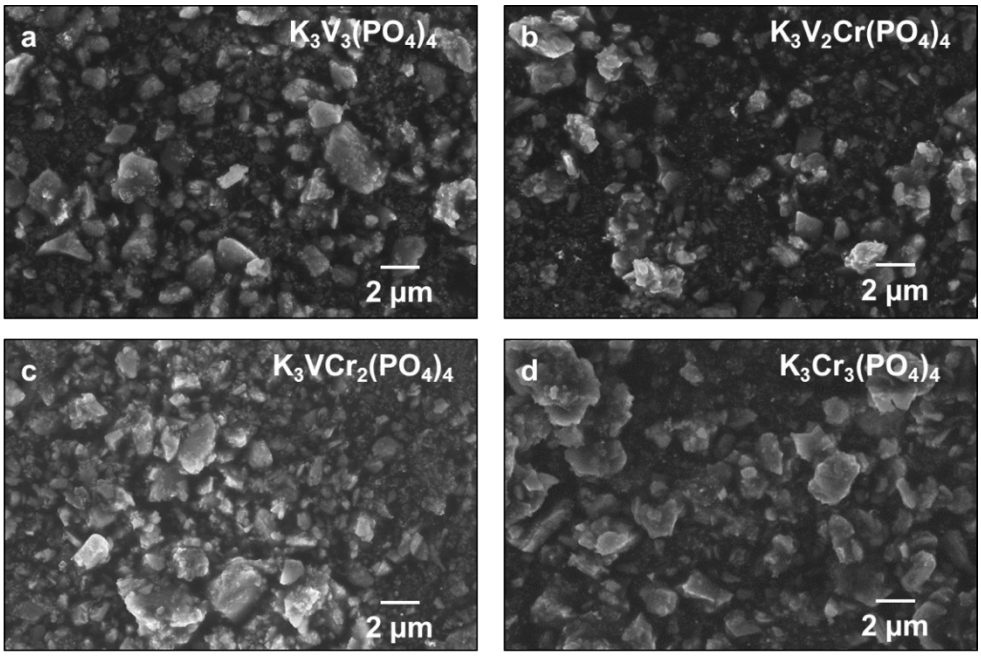

Figure S5. SEM images of **a.** $K_3V_3(PO_4)_4$, **b.** $K_3V_2Cr(PO_4)_4$, **c.** $K_3VCr_2(PO_4)_4$, and **d.** $K_3Cr_3(PO_4)_4$.

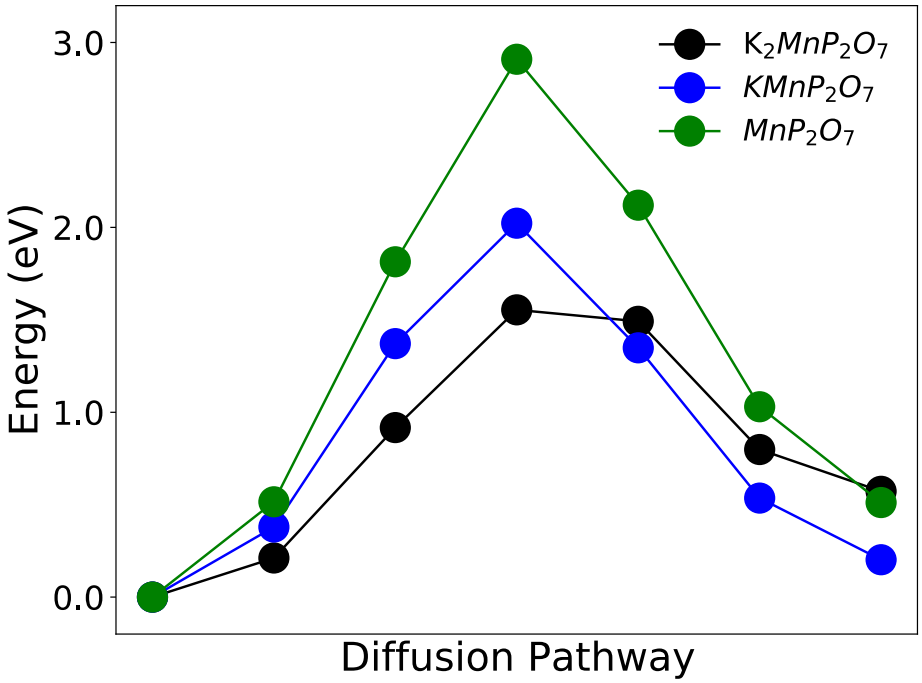

Figure S6. The energy change associated with K^+ diffusion in the $K_xMnP_2O_7$ structure calculated through Nudged Elastic Band (NEB) method.