Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A. This journal is © The Royal Society of Chemistry 2020

Electronic Supplementary Information (ESI)

Valence-to-core X-ray Emission Spectroscopy of Vanadium Oxide and Lithiated Vanadyl Phosphate Materials

Evan P. Jahrman¹(ж), William M. Holden¹, Niranjan Govind²(†), Joshua J. Kas¹, Jatinkumar Rana³, Louis F. J. Piper^{3,4}, Carrie Siu⁵, M. Stanley Whittingham⁵, Timothy T. Fister⁶, and Gerald T. Seidler¹(‡)

¹Physics Department, University of Washington, Seattle, WA 98195-1560, United States ²Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA 99354, United States

³Physics Department, Binghamton University, State University of New York, Binghamton, New York 13850, United States

⁴Materials Science and Engineering, Binghamton University, State University of New York, Binghamton, New York 13850, United States

⁵NorthEast Center for Chemical Energy Storage, Binghamton University, State University of New York, Binghamton, New York 13850, United States

⁶Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439, United States

(x) evan.jahrman@nist.gov - author is currently at the National Institute of Standards and Technology in Gaithersburg, MD; (†) niri.govind@pnnl.gov; (‡) seidler@uw.edu

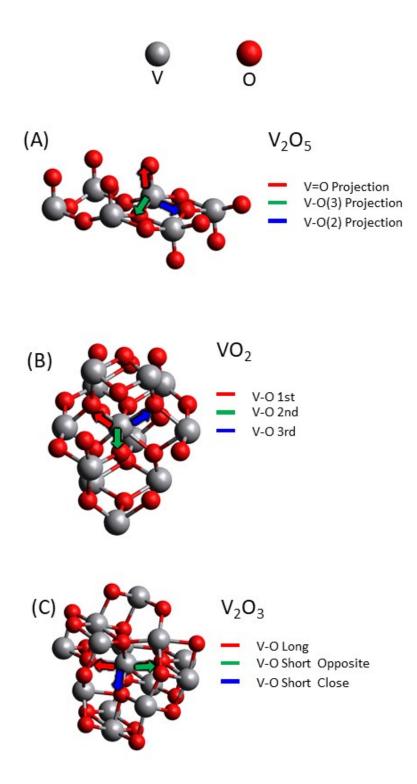


Fig. S1: A small number of atoms was extracted from the structure of V_2O_5 (a), VO_2 (b), and V_2O_3 (c). For a central V atom, three arrows are drawn to show the direction the projections were taken in Fig. 7 in the body of the manuscript. The color of these arrows matches the colors used in the legend on the right of each subpanel. Note that the small size of these groups is intended to aid visibility and is not related to the size of the clusters used in calculations.

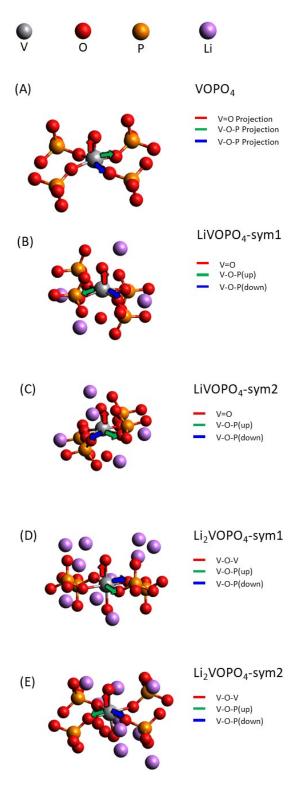


Fig. S2: A small number of atoms was extracted from each of the above structures. For a central V atom, three arrows are drawn to show the direction the projections were taken in Fig. 8 in the body of the manuscript. The color of these arrows matches the colors used in the legend. Note that the size of these groups is not related to the size of the clusters used in calculations.