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Solid state electrochemical studies on single crystals with hexafluoro metal centers[1] QIFAN YUAN, YAO ZHANG, SARAH TRUE, VICTORIA SOGHOMONIAN, Virginia Tech — Electrochemical energy storage is of importance for current and future storage schemes. Our electrochemical studies on hydrothermally synthesized single crystals of metal hexafluoride, $[NH_4]_3[V_xM'_{1-x}F_6]$, probe the redox chemistry of the V center as a function of substitution, temperature, and contact configuration. The various compositions are probed by XRD and IR spectroscopy. The measured 2 and 4 point resistivity is around 10^7 Ω cm. Cyclic voltammograms were obtained by both 2 and 3 point geometries, and current peaks corresponding to the electrochemical reaction recorded. To understand the observed voltammograms of the various configurations measured, the potential distribution in the crystal is calculated numerically, and equipotential lines extracted. Preliminary analysis indicates the extent of the space charge for 2 versus 3 contact measurements, and the influence of the space charge region on the electrochemical reaction when performed at micron scales. For a fixed sweep rate, the amplitude of the current peak diminishes as the temperature is increased, suggesting a dissipation of the space charge.

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