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The Li-induced Conversion Reaction of Ultra-Thin FeF2 Films[1]

RYAN THORPE, SYLVIE RANGAN, ROBERT BARTYNSKI, OZGUR CELIK, LESZEK WIELUNSKI, Rutgers University — Iron (II) fluoride has recently gained interest as a possible cathode material in Li-ion conversion batteries. Conversion materials like this could potentially store 2-3 times more energy than conventional intercalation battery materials by utilizing the full range of charge states in their constituent transition metal ions, i.e., $Fe^{(2+)}F_2 + 2Li^+ + 2e^- \rightarrow Fe^0 + 2LiF$. Using surface science techniques, we are able to observe this reaction at the FeF_2-Li interface. We have grown 5nm films of high-purity polycrystalline FeF_2 in ultra-high vacuum and deposited atomic Li on the surface to simulate the conversion reaction in the absence of external contaminants. Using UV photoemission (UPS), x-ray photoemission (XPS), and inverse photoemission (IPE) spectroscopies, we have measured the composition and charge states of these materials. XPS of the FeF_2 sample after various Li exposures indicate a direct conversion from Fe^{2+} to Fe^0, with no intermediary phases. The growth of a Fermi edge in UPS and IPE also indicates the formation of metallic Fe, while peaks characteristic of LiF can be seen in UPS after sufficient Li exposure. These results are consistent with those of recent TEM measurements on real electrochemical cells.

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