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Model conversion reaction: Li reactivity on iron oxifluorides SYLVIE RANGAN, RYAN THORPE, OZGUR CELIK, ROBERT BARTYNSKI, Rutgers University — Iron fluorides have gained interest as choice materials for conversion reaction-based batteries. Owing to their large band gaps and their ability to store up to three electrons per formula unit, batteries using these materials operate at high voltages and high energy densities. However the large band gap inhibits charge conduction and thus impedes efficient charging and discharging cycles. Two paths have been taken to overcome this limitation: 1) The use of nanoparticles embedded into a conducting carbon matrix improves both ionic and electronic conduction; and 2) The use of iron oxifluorides, which are characterized by a slightly reduced energy gap that facilitates electronic conduction. It is the latter point that that is central to this study as, curiously, relatively little is known about the electronic structure of iron oxifluorides and their interaction with Li, a key aspect of a storage cell's electrochemistry. Model conversion reactions have been studied by evaporating Li on FeF_2 and FeF_xO_y samples. Using X-ray and UV photoemission as well as inverse photoemission spectroscopies, the occupied states and the unoccupied electronic states of the resulting samples have been probed. Transmission electron microscopy has been used in parallel to investigate phase analysis.

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