Interphases and interfaces: SEI structure and chemical composition at silicon electrodes by ToF-SIMS and XPS Kjell Schroder*, Anthony Dylla, Hugo Celio*, Lauren J. Webb*, Keith J. Stevenson* *Texas Materials Institute, Center for Nano- and Molecular Science, and Dept. of Chemistry, The University of Texas at Austin 1 University Station Austin, TX 78712

The massive volume expansion of silicon during lithiation leads to mechanical degradation with cycling and increases electrode surface exposed to electrolyte. As a consequence, increased electrode surface area exacerbates lithium consumption by solid-electrolyte interface (SEI) forming reactions in silicon materials. We employ desiccated and anoxic techniques to prevent air and moisture contamination that allow for more accurate characterization of SEI chemical composition and stratification by XPS (1) and ToF-SIMS (Fig. 1). Results show the effect of different electrochemical treatments and surface chemistry on the composition of oligomeric and inorganic SEI products. Furthermore, we propose that conversion reactions play an important role in the formation of a true mixed oxide interphase within the SEI that affects lithiation of silicon.



Figure 1: Poisson corrected 2D intensity maps of C_2 - and F- ion fragments showing the localization of chemical species in SEI formed on (100) silicon wafer. Exposure to ambient CO₂, O₂ and moisture leads to a change in the chemical distribution of products.

REFERENCES

1. K. W. Schroder, H. Celio, L. J. Webb, and K. J. Stevenson, *J. Phys. Chem. C* **2012** *116*, 19737–19747.