Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Effect of functionalization on the electronic and atomic properties of layered MXenes KURT FREDRICKSON, Stanford University, ALEKSANDRA VOJVODIC, SLAC National Accelerator Laboratory, JENS NRSKOV, Stanford University — MXenes (M = Transition Metal, X = C or N) are a promising family of materials that have been recently manufactured from MAX phases. MXenes have already been shown as promising candidates for use in lithium ion batteries, supercapacitors, and fuel cells (1). MXenes consist of M_(x)X_(x-1), two-dimensional sheets weakly bound by van der Waals forces. However, due to the selective removal of the A ion to manufacture MXenes, they are highly reactive, with a wide variety of possible functional groups. Previous studies have shown that the electronic properties of MXene single sheets are highly dependent on their functionalization, but so far there are few studies on the effect of functionalization of the bulk phase of MXene, which consists of many layers of MXenes bound together. In this talk, we will illustrate the effect of functionalization of bulk MXenes by H, H_2, OH, and O for Mo_2C and Ti_2C. We will also show the effect of applied potential on the functionalization of Mo_2C and Ti_2C. Finally, we will compare our results with experimental measurements. (1) M. Naguib, V.D. Mochalin, M.W. Barsoum and Y. Gogotsi, *Adv. Mater.* **26**, 992 (2014).

Kurt Fredrickson
Stanford University

Date submitted: 24 Nov 2015 Electronic form version 1.4