Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Two-dimensional, ordered, double transition metals carbides (MXenes) PAUL KENT, Oak Ridge National Lab, BABAK ANASORI, Drexel University, YU XIE, Oak Ridge National Lab, MAJID BEIDAGHI, Drexel University, JUN LU, Linkoping University, Sweden, BRIAN HOSLER, Drexel University, LARS HULTMAN, Linkoping University, Sweden, YURY GOGOTSI, MICHEL BARSOUM, Drexel University — We use[1] density functional theory to predict the existence of two new families of 2D ordered carbides (MXenes), M'$_2$M"C$_2$ and M'$_2$M"$_2$C$_3$, where each M is a different early transition metal. Synthesizing $Mo_2TiC_2T_x$, $Mo_2Ti_2C_3T_x$, and $Cr_2TiC_2T_x$ (where T is a surface termination), we validated the DFT predictions. Since the Mo and Cr atoms are on the outside, they control the 2D flakes' chemical and electrochemical properties. The latter was proven by showing quite different electrochemical behavior of $Mo_2TiC_2T_x$ and $Ti_3C_2T_x$. This work further expands the family of 2D materials, offering additional choices of structures, chemistries, and ultimately useful properties. [1] B. Anasori et al. ACS Nano **9** 9507 (2015). DOI: 10.1021/acsnano.5b03591

Paul Kent
Oak Ridge National Lab

Date submitted: 05 Nov 2015 Electronic form version 1.4