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Defects in Monolayer Titanium Carbide ($Ti_3C_2T_x$) MXene XIAHAN SANG, YU XIE, MING-WEI LIN, Oak Ridge National Lab, MOHAMED ALHABEB, KATHERINE VAN AKEN, YURY GOGOTSI, Drexel University, PAUL KENT, KAI XIAO, RAYMOND UNOCIC, Oak Ridge National Lab — Mxene materials, transition metal carbides or nitrides, have recently gained interest as a developing class of 2D materials with applications geared towards energy storage, catalysis, and electronic devices. To better understand the physiochemical and electronic properties, detailed atomic resolution structural analysis of monolayer MXene was investigated using a combination of aberration-corrected scanning transmission electron microscopy, electron energy loss spectroscopy, and density functional theory (DFT). Large area $Ti_3C_2T_x$ MXene flakes, were synthesized and the type and concentration of atomic scaled defects were analyzed. Ti vacancies and Ti vacancy clusters were found to be the most prevalent defects. The edge defects, although not intrinsic to the single-layer flakes, can be created using beam irradiation. The formation energy and electronic structure of point defects and edge defects have been calculated using DFT. The influence of the defects on the conductivity is also studied using DFT. Our results thus shed light on the future nano-electronic application using 2D metallic MXene single layers.

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