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Materials Science and Engineering
College of Engineering

Department of Materials Science and Engineering
PhD Thesis Defense

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On the Electronic and Transport Properties of 2D Transition Metal Carbides and Carbonitrides (MXenes)

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Since their discovery reported in 2011, two-dimensional (2D) transition metal carbides, carbonitrides and nitrides, known collectively as MXenes, have shown promises in applications ranging from energy storage, to electromagnetic interference (EMI) shielding, transparent electrodes, optoelectronics, wireless communication, and sensors to name a few. Exceptional performances in the aforementioned applications are enabled by MXenes' high electronic conductivity, that is metallic in nature. In addition, they have a wide range of optical properties, show easy processability and high mechanical strength. Because of a large variety of chemical compositions including solid solutions, structural variations, and rich surface chemistry, MXenes are subject to multi-level manipulation of their properties, which is their unique advantage compared to majority of other bulk or 2D materials. However, the level of understanding of how the structure and composition of MXenes affect their electronic and transport properties is still insufficient.

This dissertation aims to establish relationships between MXenes' electronic properties and the intercalants, transition metals, X elements, and surface terminations with an overarching goal of demonstrating an ability to control MXenes' electronic and transport properties by controlling their structure and chemical composition. My work shows that large organic intercalants cause an expansion of the interlayer spacing and hence higher resistivity of MXenes and alter the low-temperature transport behavior. Furthermore, removal of OH- and F- surface terminations results in a lower resistivity and more than 1 eV shift of the work function in $Ti_3C_2T_x$. Moreover, replacing approximately half of the carbon atoms in $Ti_3C_2T_x$ with nitrogen atoms, forming Ti_3CNT_x, leads to lower electronic conductivity due to lower carrier mobility. Finally, magnetism introduced into a MXene *via* manipulation of the transition metal layers has been shown to strongly affect magnetotransport properties of $Cr_2TiC_2T_x$ MXene. This work paves the way toward a better understanding of MXenes' structure, processing, property, and performance relationships, focusing on electronic and transport properties as well as the realization of MXenes for high-performance optoelectronic devices and 2D heterostructures.