DREXEL UNIVERSITY
Materials Science and Engineering
College of Engineering

Department of Materials Science and Engineering,

PhD Defense

June 3rd, 10am – 12pm
LeBow 241

Electronic and Magnetic Properties of Double Metal MXenes

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Abstract

MXenes are a rapidly-expanding family of 2D transition metal carbides and nitrides with the general chemical formula of $M_{n+1}X_nT_x$, where M is one or more early transition metals, X is carbon or/and nitrogen, and T_x represents surface species. The freedom over the chemical composition of MXenes is an enabling factor in their wide range of applications such as supercapacitors, EMI shielding, catalysts, and water deionization. This dissertation focuses on fundamental electronic properties with emphasis on understanding how the M-site affects the MXene electronic behavior in three different types of double-M MXenes. The first type is out-of-plane ordered $M'_2M''C_2T_x$. The contributions of surface (M' site) and sub-surface (M" site) Ti atoms to the electronic structure are probed using soft x-ray absorption spectroscopy, revealing minimal changes in the spectral features between the parent MAX phase and its MXene when no surface Ti atoms are present in the MXene. This result indicates that the effect of T_x atoms on the electronic structure derived from sub-surface M-site layers is much less than that of surface M-site atoms. The second type is solid solution MXene $Ti_yNb_{2-y}CT_x$ where Ti and Nb are randomly ordered in the M site. To understand the intrinsic and extrinsic contributions to the macroscopic electronic transport properties, a systematic study controlling compositional and structural parameters were conducted with solid solution $Ti_yNb_{2-y}CT_x$ system. In particular, the different roles played by M-site composition, flake size and *d*-spacing on macroscopic transport is investigated via a statistical analysis. Hard x-ray photoemission spectroscopy is employed to identify changes to electronic structure induced by the M-site alloying. The third system investigated is secondary metal incorporated $Ti_3C_2T_x$ (M-$Ti_3C_2T_x$). Ni and Co are incorporated into delaminated $Ti_3C_2T_x$ by mixing dilute $NiCl_2$ or $CoCl_2$ solutions with delaminated $Ti_3C_2T_x$ solutions. DC magnetization measurements confirm that the room temperature magnetic susceptibility for Ni-Ti_3C_2 is 10 times larger than the d-Ti_3C_2, and Co-Ti_3C_2 is 100 times larger than the d-Ti_3C_2. The work provides a straightforward means of enhancing magnetic responses of MXenes using post-synthesis incorporation of magnetic transition metals.