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Exploration of Raman Spectroscopy Applications Beyond $Ti_3C_2T_x$ MXene

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Abstract

The MXene family has been rapidly expanding, with over 50 compositions synthesized to date, and hundreds of structures predicted with varying transition metals, surface terminations and carbon/nitrogen contents. While $Ti_3C_2T_x$ is the first and the most explored MXene, the search for novelty drew the attention to other MXenes that would outperform $Ti_3C_2T_x$ in various applications, such as EMI shielding, energy storage, catalysis, and biomedical applications. The performance of a device cannot be optimized without establishing the structure-property-performance relationship, which requires adequate characterization. Within the field of 2D materials, Raman spectroscopy became one of the most impactful and widely used tools: it is fast, non-destructive, offers high resolution, provides structural and electronic information, and is usable at both small-scale research and large-scale manufacturing. The goal of this thesis is to explore Raman spectroscopy characterization of MXenes beyond $Ti_3C_2T_x$ and MXene-based systems, understanding how the structure and composition of the materials affect the vibrational spectra and elucidating charge storage mechanisms of electrochemical cells in situ. For that, experimental and computational data is required. Additionally, the application of MXenes as surface-enhanced Raman spectroscopy substrates for sensing is explored. These findings will expand the usage of Raman spectroscopy by the MXene community for the characterization of MXenes. Once the strong background of the Raman spectroscopy technique is established, better, more reliable MXene devices can be engineered.