INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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SHORT ABSTRACT

With the advent of quantum information processing, and rising demand of energy-efficient, fast memory devices, spin-based technological innovation has become state of art. Magnetism, the fundamental science behind the success of such innovations, has therefore taken the centre stage of current day materials research. As components have shrunk in size and the need for high-speed, low-energy, and non-volatile functionalities has grown, researchers have been looking for materials that demonstrate magnetic properties that can be adjusted at smaller scales. The unique electrical properties and thin atomic layers of two-dimensional (2D) materials make them outstanding in this field. Because of their chemical diversity, structural adaptability, and ease of surface modification, MXenes—a broad family of 2D transition metal carbides, nitrides, and carbonitrides—have drawn attention. Initially recognized for their exceptional capabilities in energy storage and shielding against electromagnetic interference, recent theoretical and experimental studies have revealed their considerable potential in the domain of magnetism research. Their ability to support intrinsic and induced magnetism, excellent electrical conductivity, and mechanical strength make MXenes strong candidates for magnetic applications. However, the research on magnetism with MXenes is still in its infancy.In this thesis, we try to achieve two things: first, to explore the structure-property relationships in intrinsically magnetic MXenes, and second, to investigate how other traits of non-magnetic MXenes can be utilised for magnetism-related applications. Our investigation starts with studying i-MXenes, a class of in-plane chemically ordered MXenes whose MAX phase precursors have already been synthesized. We show these systems possess tunable magnetic behavior strongly influenced by surface terminations and compositional ordering. Subsequently, the magnetic and electronic properties of nitride-based MXenes with unconventional stacking sequences are explored. This study reveals how variations in stacking can substantially alter the magnetic ground state and finite-temperature behavior, introducing a novel route to tailor material properties through structural engineering.Next, we attempt to investigate multiferrocity using MXene/TMDCs heterostructure. We have shown that our heterostructure possesses magnetoelectric coupling, where ferroelectric polarization in the MXene layer can control the spin polarization in the adjacent TMDC layer. Such systems hold potential for non-volatile memory technologies and electric-field-controlled spintronic devices. Finally, we investigate the role of spin-orbit coupling (SOC) in non-centrosymmetric, non-magnetic MXenes Ta_2CS_2. We find the emergence of Rashba-like spin splitting and valley-dependent Zeeman effects arising from broken inversion symmetry and strong SOC.