

Thesis Title: Development of Two-Dimensional Magnetic Transition Metal Tellurides for Energy Applications

Abstract

Transition metal di-chalcogenides (TMDCs) compose of both layered and non-layered materials. The layered materials can be easily cleaved into atomically thin layers from bulk crystals as they have weak van der Waals binding in between them. The cleaving process can also be extended for materials with a higher c/a ratio and are non-layered. Mechanical forces and acoustic vibrations are the two most common synthesis techniques employed to form two-dimensional (2D) structures. Amongst them Tellurium has a high atomic number ($Z = 52$) and exhibits large spin-orbit coupling, due to which the properties displayed by metal tellurides differ from their sulfide and selenide counterparts. The larger ionic radius and broader d-bands in tellurides results in smaller bandgaps. They easily form metal – metalloid complexes and are comparatively less toxic in nature.

Magnetism in two-dimensional structures is as intriguing property that results in varied magnetic behaviors when thin downed to the atomic level. According to Merwin - Wagner theorem, for a 2D material, it is difficult to have long range magnetic ordering ($d \leq 3$). Magnetic anisotropy (MAE) plays a major role in long range ordering at atomic levels. Extrinsic 2D magnetic materials which originate from external stimuli such as doping and strains find various room temperature applications. In this work we extend to explore few compositions of 2D transition metal tellurides (TMTs) consisting of manganese and chromium metal complexes (MnTe , MnTe_2 , Cr_2Te_3 and CrTe_3). Multiple magnetic phase transitions were observed in the 2D material, which can help tune bandgap. The distance between atoms was varied via elastic strain, which is not possible in bulk structures. We observe shifts in Curie temperature (T_c) and Neel Temperature (T_N) which is due to change in lattice structure. This is due to unbalanced spin majority and increased spin populations.

We find applications of these 2D TMTs in room temperature spintronic application, observed non - thermal deicing due to ferromagnetic to paramagnetic transitions at room temperature, for energy efficient photodegradation of dyes and also explored their charge generation capabilities devising Flexible Nanogenerators.