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Understanding the magnetic and electronic properties of transition-metal chalcogenides T. LAMARTINA, Univ of North Florida, A.V. BALATSKY, Los Alamos National Laboratory/NORDITA, J.T. HARALDSEN, Univ of North Florida — This study computationally examines the magnetic and electronic properties for various transition-metal chalcogenides (M_2X_2 with M = Cr, Mn, Fe, and Co and X = S, Se) using density functional theory. The M_2X_2 structure is a quasi two-dimensional honeycomb lattice. Through spin-polarized general gradient approximation with onsite potential (SGGA + U), we determine and compare the net electronic structure and density of states for the various compounds. Examination of the net magnetic moment and structure suggest a distorted tetrahedral crystal-field symmetry, and an analysis of the electronic structure shows the presence of nodal points that resemble Dirac nodes. Overall, it is predicted that all materials demonstrate a ferromagnetic metallic state, while some structures (mainly Cr-based) have a half-metallic state. This leads to the possibility of Dirac half-metal states.

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