Spin transport properties of $zCrX_2$ (X = S, Se) nanoribbons

Frank Hagelberg

Department of Physics and Astronomy, East Tennessee State University

Transition metal dichalcogenides (TMDCs) form stacked compounds from 2D sheets of composition TMX_2, consisting of transition metal (TM = Ti, V, Cr, Tc, Hf, Ta, W, Mn, Zr, Nb, Mo, Re) monolayers sandwiched by two chalcogen (X =S, Se, Te) monolayers. TMDCs share various features with graphene but have a bandgap in the optical regime. Most TMDCs have turned out to be non-magnetic [X. Song et al., Appl. Phys. Rev. 8, 011312 (2021)]. Dimensional reduction from 2D-materials to nanoribbons, however, may induce magnetism in these systems. Recently, the first fabrication of chromium dichalcogenide was announced [Shivayogimath et al., Nat.Comm. 10, 2957 (2019)] which may exhibit magnetic phases [M. R. Habib et al., Nanoscale 11, 20123 (2019), K.Chen et al., NPJ Comp.Mat.7, 79 (2021)]. The present work deals with transport properties of CrS_2 nanoribbons of the zigzag type (zCrS2), with special emphasis on properties of potential interest for nanospintronics. Specifically, the magnetoresistance and spin filtering properties of $zCrS_2$ ribbons with five CrS_2 rows (5-$zCrS_2$) were investigated by density functional theory (DFT) in conjunction with a Green's Function procedure. In the bias regime V < 10 mV, magnetoresistance ratios in the order of 10^6 % were obtained, and half-metallicity was established for the magnetic ground state of 5-$zCrS_2$, associated with magnetocurrent ratios of 100 %. Applying gate fields to the ribbon turned out to be a way of controlling the sign of the spin population emerging from 5-$zCrS_2$.