Spin Transport through Nanoribbons based on Transition Metal Dichalcogenides (TMDCs): Implications for Spintronics

Frank Hagelberg , Robert B. Yeatts

Department of Physics and Astronomy, East Tennessee State University,
Johnson City, TN 37614, USA

The challenge of miniaturizing spintronics is at the frontier of present-day nanoscience [Jour.Phys.:Condens.Mat. 19, 165222 (2007)]. It involves shrinking the elements of spintronics networks, such as spin valves, spin filters, spin diodes, and spin transistors, to the nanoscale. Low-dimensional structures, such as magnetic monolayers and nanoribbons are instrumental for reaching this goal. Computational as well as experimental research at the intersection between nanomagnetism and spintronics has primarily focused on graphene and graphene derivatives. Among other 2D-nanostructures that have been suggested as potential building materials for elements of nanospintronics are transition-metal dichalcogenides (TMDCs) [Nat. Rev. Mat., 2, 17033 (2017)]. The purpose of the present study is to explore zigzag nanoribbons based on the recently characterized TMDC species CrS_2 [Nat.Comm. *10*, 2957 (2019)] with respect to their spin transport properties. More specifically, density functional theory (DFT) in conjunction with a non-equilibrium Green's Function (NEGF) approach is used to model the magnetoresistance and spin filtering properties of $zCrS_2NRs$ with five CrS_2 rows (5-$zCrS_2NRs$) as a function of longitudinal strain as well as vertical and lateral gate fields for ferromagnetic (FM) and antiferromagnetic (AFM) phases of the ribbon. In the bias regime $V < 10$ mV, magnetoresistance ratios up 10^7% are obtained, and half-metallicity is established for the magnetic ground state of 5-$zCrS_2NR$ (AFM), associated with magnetocurrent ratios of 100%. Applying lateral gate fields to the ribbon turns out to be a way of controlling the sign of the net spin population emerging from 5-$zCrS_2NR$. Furthermore, we examine the dependence of our results on the chalcogen species by analyzing the units 5-$zCrSe_2NR$ and 5-zCrSeSNR. Emphasis is placed on the latter which is derived from a Janus TMDC, an asymmetric structure comprising a transition metal layer sandwiched by two different chalcogen layers. Specifically, we interpret the spin transport properties of the Janus ribbon in terms of our findings on strained and laterally gated $zCrS_2$ ribbons.