# Spin-valley transport in magnetic 2D materials through multiscale simulations

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## Introduction

Recently, two-dimensional (2D) magnetic materials have attracted great attention for their magnetic, electrical and physical properties that can open new paths for the design of nanoscale spintronic and valleytronic devices [1]. In particular, bilayer $CrI_3$ outstands for its antiferromagnetic ground state and with weak interlayer coupling which allows to switch the magnetic ground state by applying an external electric field [2]. In addition, the possibility to interface 2D magnetic materials with other van der Waals materials such as transition metal dichalcogenides has opened new possibilities for the observation of new and exciting physical phenomena. Here we present two proof-of-concept devices, a double split-gate device based on bilayer $CrI_3$ and then a valleytronic device based on $CrBr_3$-encapsulated $WSe_2$.

## Method

In order to investigate the proposed device concept and evaluate its performance as a spin-valve transistor, we use a multiscale approach combining *ab-initio* DFT calculations, using Quantum Espresso suite [3], maximally localized Wannier functions [4] and non-equilibirum transport calculations using the Green's functions approach. The transport through the devices is solved self-consistently with the device electrostatics using the NanoTCAD ViDES [5] device simulation code.

## Discussion

The first device based on bilayer $CrI_3$ is reported in Fig. 1 (top). The first two gates ($V_{g1}$) act as control electrodes for the spin filtering, selecting either spin-up or spin-down carriers depending on the electric field orientation, while the second two gates ($V_{g2}$) turn ON and OFF the selected spin current, effectively acting as a spin detector as schematically depicted in Fig. 1 (bottom). In Fig. 2 we present the spin-polarized current (a) and difference between the $I_{up}$ and the $I_{down}$ (b) for different values of $V_{g1/2}$, demonstrating the tunability of the spin-polarized current through gates. The second device is presented in Fig. 3 and it is based on $CrBr_3$/$WSe_2$/$CrBr_3$ van der Waals trilayer heterostructure. It leverages on the valley splitting that takes place in the conduction band of $WSe_2$ due to the hybridization with the spin-polarized bands of the $CrBr_3$ layers. The valley splitting can be controlled through the relative orientation of the magnetization in both $CrBr_3$ layers, leading to K, K' , or 0 valley-polarized devices (Fig, 4).

## Conclusion

We have presented two proof-of-concept devices, a double split-gate device which is able to both filter ($> 99\%$) and select ON/OFF the spin current up to a ratio of $\approx 10^2$, based on bilayer $CrI_3$ and a valleytronic device based on $CrBr_3$-encapsulated $WSe_2$. The latter shows an unprecedented valley splitting of $\sim 100$ meV, able to be tuned by the relative magnetization of the encapsulating layers.

## Acknowledgment

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## References

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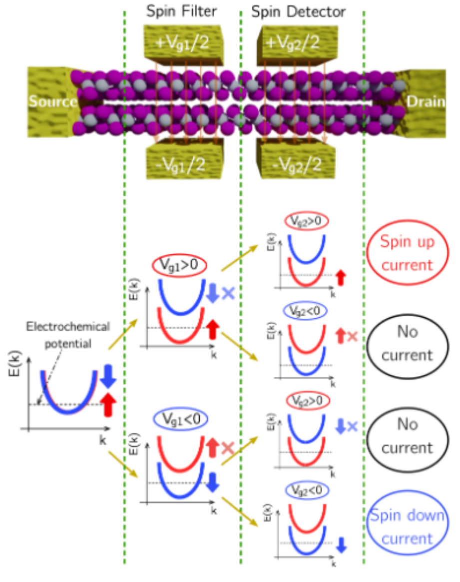



Fig. 1. (Top) Schematic of the device architecture. (Bottom) Pictorial sketch of the spin-polarized bottom of the conduction band structure for the filtering and detecting mechanism for different values of $V_{g1}$ and $V_{g2}$.

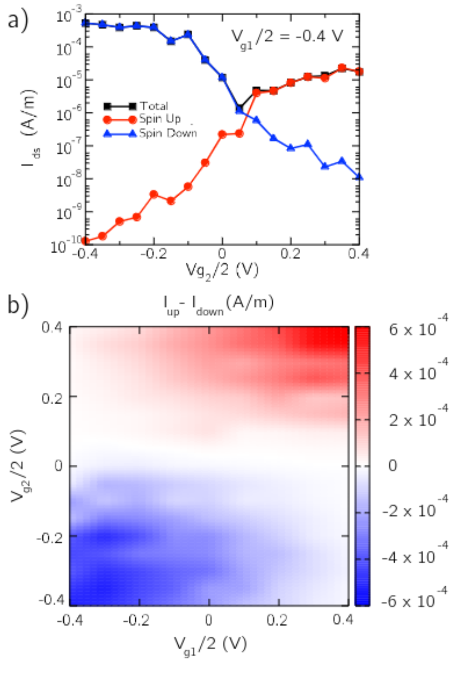



Fig. 2. Total, spin up and spin down currents as a function of $V_{g2}$ for $V_{g1}/2$ = -0.4 V. b) Color map of the difference between spin up current ($I_{up}$) and spin down current ($I_{down}$) as a function of $V_{g1}$ and $V_{g2}$.

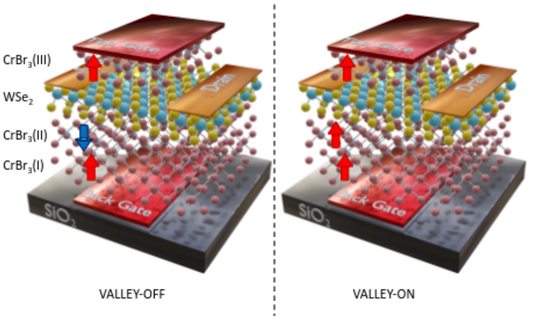



Fig. 3. Schematics of the proposed proof-of-concept valleytronic field-effect transistor.

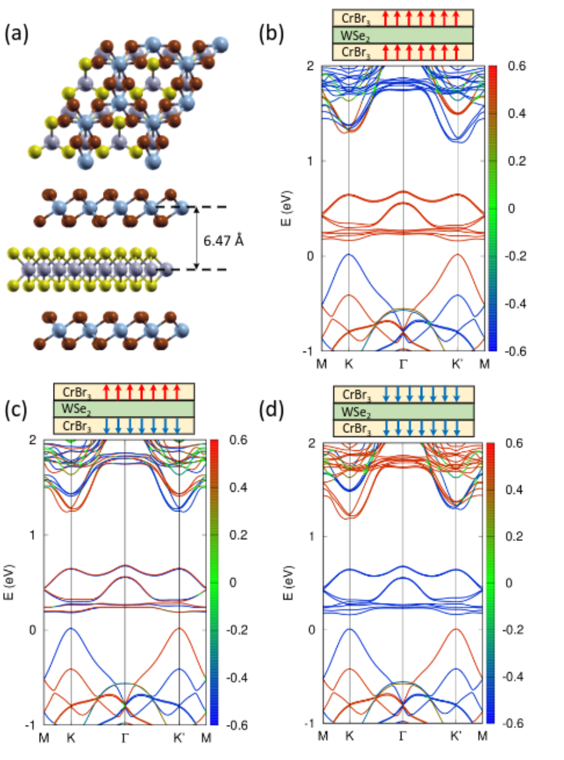



Fig. 4. (a) Details of the stacking configuration of $CrBr_3/WSe_2/CrBr_3$ trilayer heterostructure. Gray and yellow spheres correspond to W and Se atoms, respectively. Blue and brown spheres correspond to Cr and Br atoms, respectively. First-principles band structure for three different magnetic orientations: (b) $CrBr_3$ layers are co-polarized up, (c) $CrBr_3$ layers are counter-polarized, and (d) $CrBr_3$ layers are co-polarized down. Insets illustrate the magnetic configurations of the $CrBr_3$ layers in each case.