Spin transport in CrXY monolayers: multiscale computational study

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Two-dimensional magnetic materials show a high potential for spintronic devices [1] thanks to intriguing phenomena at their interfaces. Their experimental investigation, while being actively performed, poses many challenges and numerical simulations can be of great help by pin-pointing high-gain materials and guiding the experimental research [2]. In this study we use a complete set of computational techniques to assess the suitability of CrXY [X, Y ∈ {S, Se, Te}] monolayers for spintronics, focusing on spin-momentum locking, highly relevant for spin manipulation by an electric current. We start from *ab initio* calculations and create tight-binding models [3] further used to compute the exchange parameters, Curie temperature and anomalous Hall conductivity. We find spin-momentum locking of complex forms which is shown to come from higher-order terms in the in-plane momentum expansion of the spin-orbit Hamiltonian [4]. Along with the calculated structural properties and magnetic anisotropy, this allows us to draw important conclusions about the possible use of CrXY monolayers in spintronic devices.

References

[1] *B. Dieny et al., Nature Electronics **3** (2020) 446*
[2] *Q. H. Wang et al., ACS Nano **16** (2020) 6960*
[3] *A. A. Mostofi et al., Computer Physics Communications **185** (2014) 2309*
[4] *S. Vajna et al., Physical Review B **85** (2012) 075404*

Figures

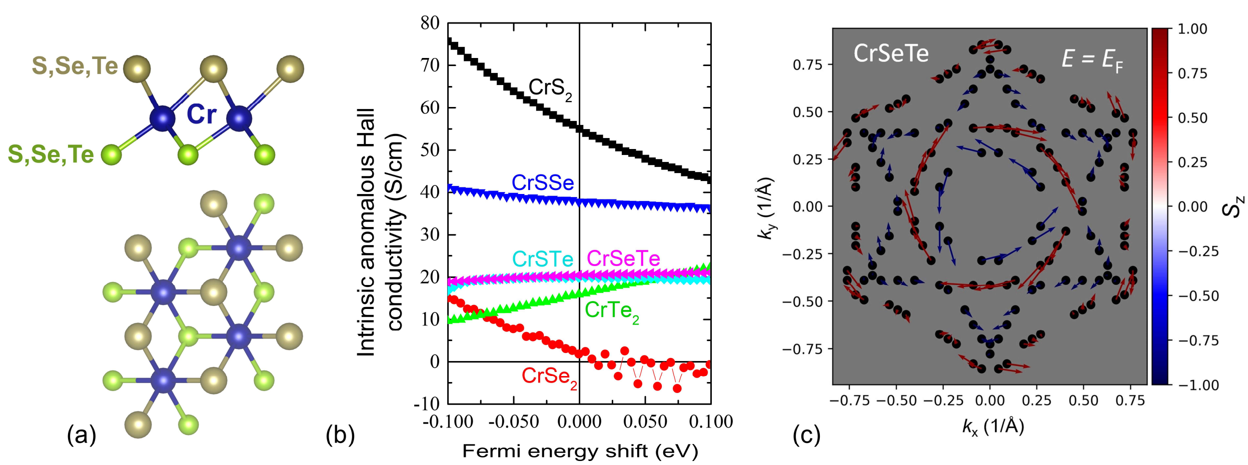

Figure 1: *Ab initio* calculations of CrXY [X, Y ∈ {S, Se, Te}] monolayers in the 1T phase. (a) Crystal structure of the monolayer 1T phase. (b) Calculated intrinsic anomalous Hall conductivity as a function of Fermi energy shift for the 6 materials. (c) Spin texture at the Fermi surface of a monolayer CrSeTe as a function of the in-plane wave vectors. The asymmetrical structure leads to an effective out-of-plane electric field and resulting Rashba-like spin-momentum locking.