Controlling the magnetic properties of monolayer $Cr_2Ge_2Te_6$ by electrostatic gating: an ab-initio study

Guido Menichetti[a,b]
Matteo Calandra[c,d]
Marco Polini[a,b,e]
[a]*Istituto Italiano di Tecnologia, P.zza S. Silvestro 12, 56127, Pisa, Italy*
[b]*Dipartimento di Fisica "E. Fermi", Università di Pisa, Largo Pontecorvo 3, I-56127 Pisa, Italy*
[d]*Dipartimento di Fisica, Università di Trento, via Sommarive 14, I-38123 Povo, Italy*
[d]*Sorbonne Université, CNRS, Institut des Nanosciences de Paris, UMR7588, F-75252, Paris, France*
[e]*School of Physics & Astronomy, University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom*
guido.menichetti@iit.it

Van der Waals materials have always been source of fascinating phenomena. In fact, the atomic thickness of two-dimensional materials provides the unique opportunity to control their electrical and optical properties[1]. The discovery of two-dimensional magnetic materials[2-4], in particular, paves the way for the electrical control of magnetism and the realization of new functional devices for spintronic applications. Therefore, the possibility of doping these few layer systems via the electric field effect is certainly very appealing.
Though most of the vdW magnets behave semiconductors, very few reports have been conducted on field effect transistors based on such magnets, in particular on CrI_3[5] and $Cr_2Ge_2Te_6$[6].
The atomic nature of 2D magnetic materials and the understanding of competing microscopic mechanisms behind the electrostatic gating in such materials is obviously rather complex and requires massive use of ab initio theories. In this work, we present an extensive analysis, based density functional theory (DFT), on the doping dependence of the magnetic properties of monolayer $Cr_2Ge_2Te_6$[7]. We first show effects of electrons/holes doping on the electronic properties on the monolayer $Cr_2Ge_2Te_6$. Then we investigate its magnetic structure with a hybrid functional[8], with super-cells containing up to 160 atoms. We evaluate the magneto-crystalline anisotropy energy, all the relevant exchange couplings showing that is possible to control the Curie temperature by electrostatic gating. We compare our results with recent available experimental data.

The research leading to these results has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement no. 881603-Graphene Core3.

References

[1] A.K. Geim and I.V. Grigorieva, Nature, 499 (2013) 419.
[2] C. Gong, L. Li, Z. Li et al., Nature, 546 (2017) 265.
[3] B. Huang, G. Clark, E. Navarro-Moratalla et al., Nature, 546 (2017) 270.
[4] M. Gibertini, M. Koperski, A.F. Morpurgo, and K.S. Novoselov, Nat. Nanotechnol., 14 (2019) 408.
[5] S. Jiang, L. Li, Z. Wang et al., Nat. Nanotechnol., 13 (2018) 549
[6] I.A. Verzhbitskiy, H. Kurebayashi, H. Cheng, et al., Nature Electronics, 3 (2020) 460.
[7] T. Brumme, M. Calandra, and F. Mauri, Phys. Rev. B, 89 (2014) 245406
[8] G. Menichetti, M. Calandra, and M. Polini, 2D Material, 6 (2019) 045042