Interplay between magnetism and topology in HgTe doped with Cr and V

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Dilute magnetic semiconductors have played a central role in the demonstrating and describing a strong and intricate influence of the sp-d exchange interactions upon effective mass states in semiconductors, paving the way for the rise of dilute ferromagnetic semiconductors [1] and magnetic topological insulators [2,3,4]. Recently the exchange splittings of magneto-optical spectra in $Cd_{1-x}Mn_xTe$ and $Hg_{1-x}Mn_xTe$ have been described [5] and it has been demonstrated that superexchange dominates in magnetic topological insulators [6]. Here we investigate the electronic and magnetic properties of the dilute magnetic semiconductors $Cd_{1-x}Cr_xTe$, $Hg_{1-x}Cr_xTe$, $Cd_{1-x}V_xTe$, $Hg_{1-x}V_xTe$ by using a density functional theory approach which goes beyond the standard functionals in order to correctly reproduce the topology and the band gap of these systems. We obtain the band structures of these systems, we study the distortions produced by the Jahn-Teller effect and the crystal field splitting of the d-levels of the dopants. We find that the crystal field strongly depends on the correlations. Then, we study the exchange couplings for all considered cases and we find that the coupling is ferromagnetic in case of doping with V, differently from the case of doping with Mn and Cr, where we find antiferromagnetic couplings. The ferromagnetic coupling among V atoms in the insulating phase of topological HgTe can produce the quantum anomalous Hall phase. We also checked the interplay between the distortions produced by Jahn-Teller effect and magnetism and we found that the distortions favor the ferromagnetism.

References:

[1] T. Dietl and H. Ohno, *Rev. Mod. Phys.* **86**, 187 (2014).
[2] H. Ke, Y. Wang, and Q.-K. Xue, *Annu. Rev. Condens. Matter Phys.* **9**, 329 (2018).
[3] Y. Tokura, K. Yasuda, and A. Tsukazaki, *Nat. Rev. Phys.* **1**, 126 (2019).
[4] R. Islam, S. Mardanya, A. Lau, G. Cuono, T.-R. Chang, B. Singh, C. M. Canali, T. Dietl, and C. Autieri, *Phys. Rev. B* **107**, 125102 (2023).
[5] C. Autieri, C. Śliwa, R. Islam, G. Cuono and T. Dietl, *Phys. Rev. B* **103**, 115209 (2021).
[6] C. Śliwa, C. Autieri, J. A. Majewski, and T. Dietl, *Phys. Rev. B* **104**, L220404 (2021).