DFT-based spin-orbit torque calculation in two-dimensional Cr-intercalated $CrTe_2$ layered transition metal halides

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Intensive studies in two-dimensional (2D) magnetic materials are due to their potential to enable improved efficiency in the electrical control of magnetic devices with energy consumption. The majority of layered magnetic material includes two families, namely, transition metal halides [1] and transition metal chalcogenides [2]. The magnetic anisotropy for most known cases are believe to be along the out-of-plane direction, however, it remains debated in Cr-intercalated $CrTe_2$ layered transition metal halides, especially from the computational point of view.

In this study, we first employ the first-principles calculation to obtain the structural, electronic, and magnetic properties of various intercalating Cr concentrations among $CrTe_2$, Cr_7Te_{12}, Cr_8Te_{12}, and Cr_3Te_4 monolayers. Our self-developed DFT-based spin-orbit torque (SOT) calculation [3, 4] is then applied to predict their magnetic anisotropies, which successfully explains the sudden drop of magnetic anisotropy energy per Cr ion in the Cr_7Te_{12} case.

Recently, Guo et al. have predicted Cr_3Te_4 as a possible room-temperature 2D ferromagnetic (FM) material [5]. We further propose a $Cr_3Te_4/PtTe_2$ van der Waals heterobilayer to investigate the current-induced SOT. Our work reveals that local spin induction significantly generates the field-like torque, which primarily governs the switching current in systems with in-plane magnetic anisotropy. This work is supported by the National Science and Technology Council (NSTC 112-2112-M-008-036).

References

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