Spin-orbit-proximitized ferromagnetic metal due to monolayer transition metal dichalcogenides: Atlas of spectral functions, spin textures and spin-orbit torques for Co/MoS_2, Co/WSe_2 and Co/$TaSe_2$ heterostructures

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The bilayer heterostructures composed of an ultrathin ferromagnetic metal (FM) and a material hosting strong spin-orbit coupling (SOC) are a principal resource for spin-orbit torque and spin-to-charge conversion effects in spintronics. The key to understand these effects is current-driven nonequilibrium spin density which appears on any monolayer of the heterostructure where SOC is nonzero. Here we demonstrate that hybridization of a wavefunction of four monolayers of Co and a wavefunction of monolayer of transition metal dichalcogenides (TMDs)—such as semiconducting MoS_2, WSe_2 and metallic $TaSe_2$—leads to drastically different electronic and spin structure of Co layer when compared to its bulk. This is due to SO splitting of its bands encoded in the spectral functions and spin textures on its monolayers, which we extract from noncollinear density functional theory (ncDFT) combined with Green function calculations. In fact, SO splitting is present due to inversion symmetry breaking by the bilayer structure even if SOC within TMD monolayer is selectively turned off, but turning it in on in ncDFT calculations makes proximity SOC within Co layers about three times larger. Passing current through nonzero spin textures on monolayer of Co generates nonequilibrium spin density within its monolayers, whose cross product with the exchange-correlation magnetic field of Co gives spin-orbit torque, and these two quantities can be used to quantify the efficiency of SOC induced in Co. In particular, this isolates WSe_2 as the most optimal choice, among the three TMDs screened, for maximizing SO proximity effect and the corresponding nonequilibrium effects for spintronic applications.

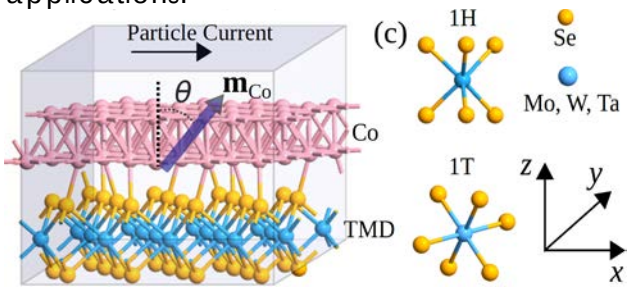

Figure 1: Schematic view of bilayers, composed of two monolayers of Co and monolayer TMD, for calculating nonequilibrium spin density and the corresponding SOT.

References

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