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Tunable magnetic interaction by an applied electric field in Co-adsorbed SiC monolayer

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Recently, many researchers have given special attention to the properties of metal adsorbed two-dimensional (2D) nanosheet. Influence of electric field (EF) on magnetic properties, such as magnetic anisotropy energy (MAE) and the spin transport, magnetic moment, has also attracted growing interests in nanosheets. In order to find its potential applications, we study the influence of an EF on Co-adsorbed SiC monolayer by using first-principles calculations. The first-principles method is based on density functional theory (DFT), which is implemented in the VASP package. In this paper, we investigate the magnetic properties of two Co atoms adsorption on SiC monolayer under an applied electric field, as shown in Fig. 1a.

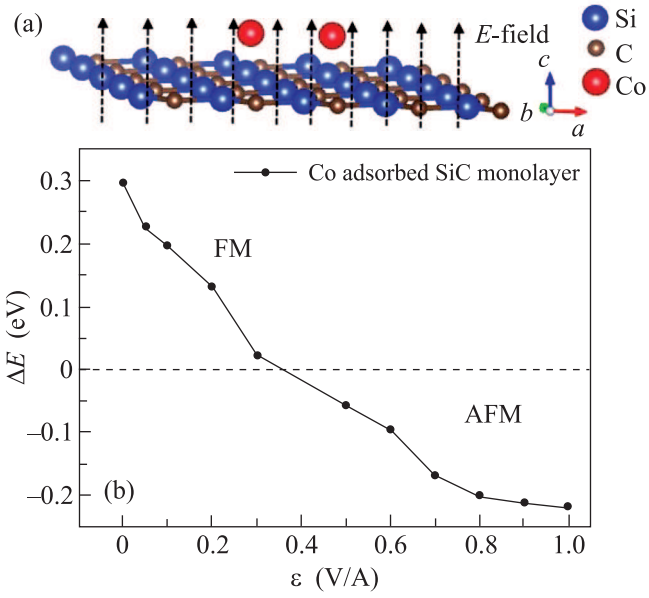

Fig. 1. (a) – Side view of two Co adsorbed $5 \times 5 \times 1$ SiC monolayer and electric field along the c-axis. (b) – The total energy difference ΔE as a function of electric field strength ε

Without an electric field, two Co atoms show the strongest ferromagnetic (FM) interaction. The polarized spins in C/Si p states couple with the d localized spins of Co, showing a p–d like interaction chain, which results in an indirect FM interaction between Co and C/Si atoms. Under an electric field, the FM interaction between two Co atoms changes to antiferromagnetic (AFM), as shown in Fig. 1b. In this situation, the superexchange takes over, destroying the ferromagnetism. Thus, the preferred magnetic coupling between two Co atoms should be AFM with null spin polarization. Moreover, the sign of the MAE doesn't changes with the increased field strength, the magnetic easy axis is always parallel to the a-axis.

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