Spin states at the edges of a finite p-orbital helical atomic chain attached to a ferromagnetic substrate

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The chiral-induced spin selectivity (CISS) effect is the phenomenon in which a chiral molecule acts as a spin filter, selecting a specific spin orientation depending on its chirality. Over the last two decades, the CISS phenomenon has been observed in various chiral molecules and has attracted considerable attention due to its significant effect, even at room temperature, despite chiral molecules not containing magnetic atoms [1]. While numerous theoretical proposals have been made, a comprehensive understanding has not yet been established. We have analyzed the CISS phenomenon based on a p-orbital helical atomic chain with intra-atomic spin-orbit interaction (SOI), which serves as a toy model of helical molecules such as DNA [2-3]. Here, we apply this model to explain an enantioselective experiment [4], which demonstrated that molecules with specific chirality preferentially adsorb onto a magnetic substrate with a particular orientation of magnetization.

In the case of an infinite chain, our model supports a spin-filtering state where two up spins propagate in one direction while two down spins propagate in the opposite direction without breaking time-reversal symmetry (TRS). For a finite chain, the presence of evanescent states induces an enhancement of charge modulations concentrated at the edges, although spin density is absent due to the preservation of TRS [2]. A Zeeman field applied at the edge of the atomic chain, mimicking the effect of a magnetic substrate, breaks theTRS and induces a finite spin polarization. The direction of this polarization depends on the chirality of the molecule. The change in chirality leads to a reasonable amount of energy difference, offering insight into the enantioselective adsorption of chiral molecules on a ferromagnetic surface [2].

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