Supporting Information

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SI Text

Spin Transport Through the Single-Stranded DNA in the Presence of Twist Angle Disorder

Fig. S1 *A* and *B* show, respectively, the spin-up conductance $G_\uparrow$ and the spin polarization P_s for the single-stranded DNA (ssDNA) in the presence of the twist angle disorder, which can be traced back to the distorted ssDNA structure. Here, the twist angle disorder may be modeled by considering the rigid sugar-phosphate backbone where both the radius R and the nearest neighbor (NN) distance l_1 are fixed (1, 2). Then, the twist angle $\Delta\varphi_n$ between the nth and $n + 1$th nucleobases is distributed in the range $[\Delta\varphi - D/2, \Delta\varphi + D/2]$ randomly and uniformly, with $\Delta\varphi$ the twist angle of the regular B-form structure and D the disorder strength. It is clear that when there exists the twist angle disorder, each nucleobase will fluctuate randomly from its equilibrium position. As a result, the ssDNA deviates from the B-form structure and the helicity of the ssDNA can somewhat be destroyed. One can see from Fig. S1*B* that the ssDNA cannot be a spin filter with the order of magnitude of the spin polarization being 10^{-5}, no matter whether the twist angle disorder is considered or not.

Spin Selectivity of the Peptide in the Region of Weak Spin-Orbit Coupling

To clearly illustrate the magnitude of the spin-orbit coupling (SOC) at which the spin-filtering effect of the peptide is still pronounced, Fig. S2*A* plots P_s for different renormalized NN SOC s_1 and Fig. S2*B* displays the averaged spin polarization $\langle P_s \rangle$ vs. s_1. It clearly appears that the spin selectivity of the peptide remains significant in the region of very weak SOC. For instance, the spin polarization can reach the value 6.4%, 10.6%, 14.2%, 27.6%, 33.7%, and 37.1% by increasing s_1 from $0.004t_1$ to $0.07t_1$ (see Fig. S2*A*).

1. Gore J, et al. (2006) DNA overwinds when stretched. *Nature* 442(7104):836–839.

2. Guo AM, Sun QF (2012) Spin-selective transport of electrons in DNA double helix. *Phys Rev Lett* 108(21):218102.
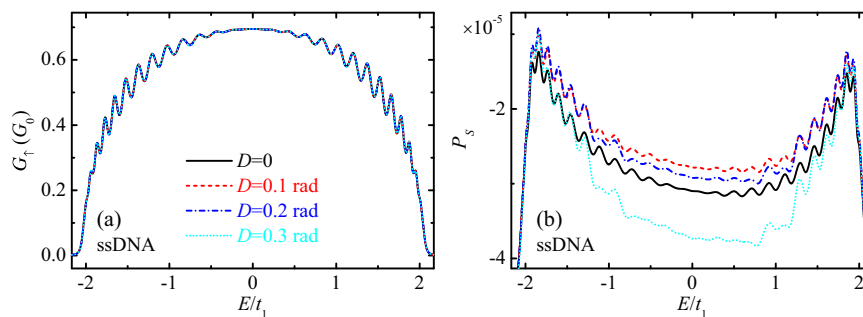
Fig. S1. Spin transport property of the ssDNA in the presence of the twist angle disorder. (*A*) Energy-dependent spin-up conductance $G_\uparrow$ and (*B*) spin polarization P_s for various strengths of the twist angle disorder. Here, $G_0 = e^2/h$ is the quantum conductance. The model parameters are $N = 30$, $s_1 = 0.12t_1$, $l_c = 0.9$ Å, and $\Gamma_d = 0.06t_1$. The results are calculated from a single disorder configuration and are similar for other disorder configurations.
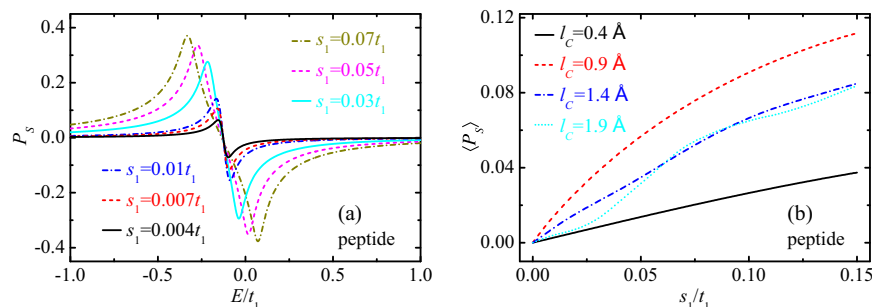

Fig. S2. Spin filtration efficiency of the peptide for various SOC strengths. (*A*) Energy-dependent spin polarization P_s with several values of the renormalized NN SOC s_1. The model parameters are $N = 60$, $l_c = 0.9$ Å, and $\Gamma_d = 0.06t_1$. (*B*) Averaged spin polarization $\langle P_s \rangle$ vs. s_1 for various decay exponent l_c with $N = 60$ and $\Gamma_d = 0.06t_1$.