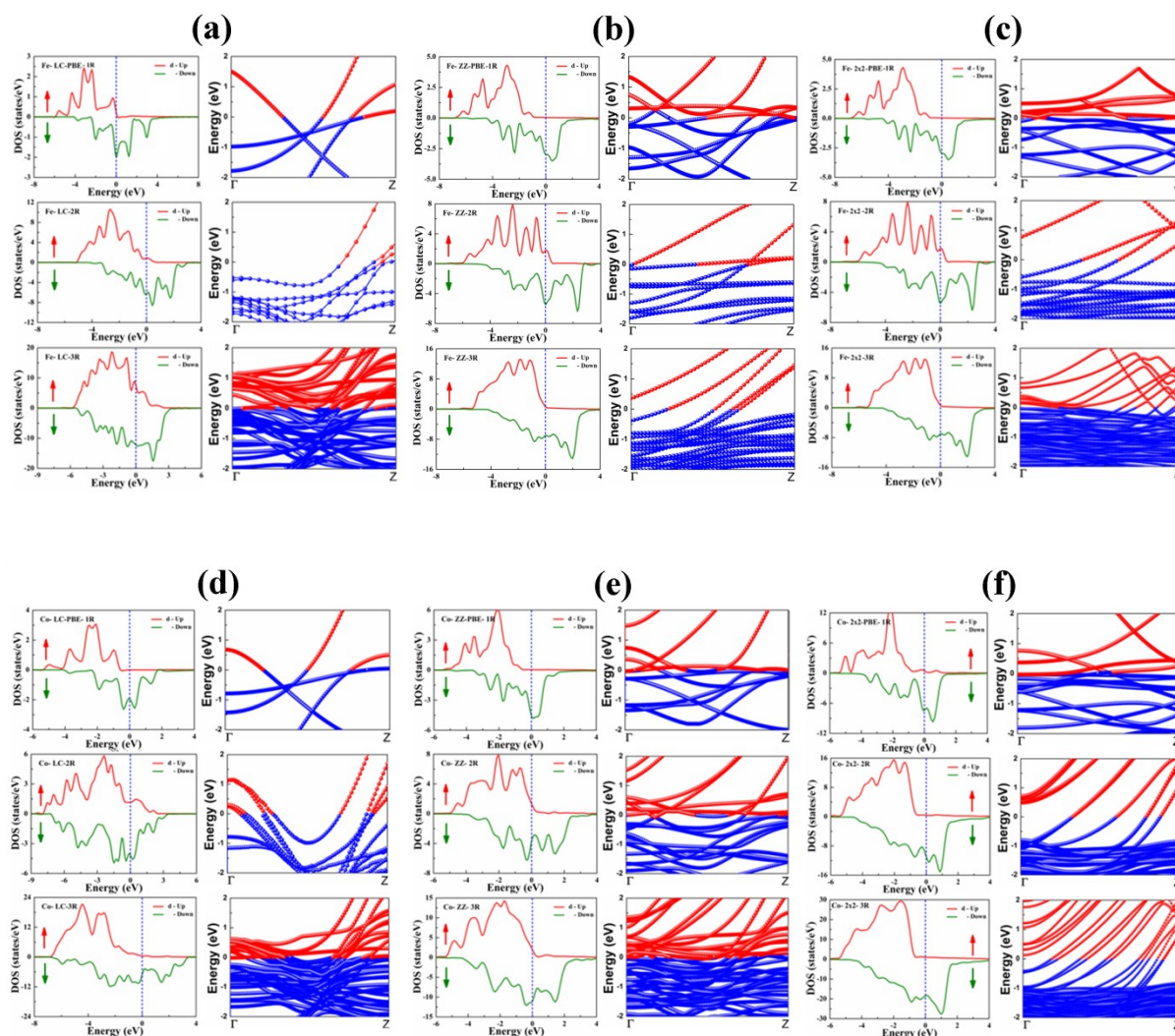# Supplementary information

Figure S1. Electronic band structure and projected density of states (PDOS) for different diameters (denoted as 1R, 2R and 3R in figure) of LCs, ZZ and 2×2 NWs without spin-orbit coupling (SOC) of Fe (a-c) and Co (d-f) atoms.

In Figure 3 of PDOS of Fe LC-1R NW, there are d orbital of up spin and down spin contribute their high possibilities in the range of -3.16 to -2.56 and -0.50 to 1.72 eV while in the part of the without SOC, no more changes are seen in the studied range of energies. In this case up spin and down spin have the highest contributions from -3.66 to -1.85 and -0.51 to 1.70 eV for 1R, -5.0 to -1.0 and -2.22 to 2.30 eV and for 3R, it is -4.5 to -0.75 and -4.5 to 3.0 eV. For the structure configuration of ZZ-1R-2R-3R, the spin up and down SOC are [-4.47, -0.80↑] [-1.52, 2.07↓], [-4.43, 1.68↑] [-3.80, 2.20↓], [-5.09, 0↑] [-2.53, 2.50↓], respectively. According to SOC, the highest peak of density of states for the 2×2- 1R structure is [9.0↑, -8.55↓], for 2R, the peak is [19. 25↑, -14.07↓] and [2.0↑, -1.88↓]. The

occupied range of up spin for 2×2 is [-5.82, -1.50]- 1R, [-5.33, -0.77]- 2R and [-5.0, -1.02] for the case of SOC and [-2.77, 1.68]-1R, [-2.56, 2.75]-2R and [-2.30, 2.80]-3R for the down spin case of SOC.

In Figure 4 of PDOS of Co NWs is describing that the highest range of density energy of states and covered the range due to their spreading. In configuration of LC, ZZ, 2×2 with 1R, 2R, 3R, the highest peaks of spin up channel meet accordingly [-3.70, -0.90]- 1R, [5.0, -0.80]- 2R, [-6.80, 2.20]- 3R for LC, [-3.52,-0.94]- 1R, [-6.20, -1.50]- 2R, [-7.60, -1.80]- 3R for ZZ and for 2×2 is [-3.87, -1.41]- 1R, [-5.20, -1.12]- 2R, [-6.00, -1.00]- 3R eV for SOC and while for down spin channel it is [-1.88, 1.35]- 1R, [-3.20, 1.10]- 2R, [-5.80, 0.30]- 3R for LC, [-2.17, 0.38]- 1R, [-2.30, 2.80]- 2R, [-2.30, 2.00]-3R for ZZ and for 2×2 is [-1.35, 0.93]- 1R, [-1.40, 0.80]- 2R, [-3.10, 0.75]-3R eV for SOC.