Supporting Information for

“2D Mn2C6Se12 and Mn2C6S6Se6: Intrinsic Room-Temperature Dirac Spin Gapless Semiconductors and Perfect Spin Transport Properties”

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Figure S1. Evolution of total energy of the Mn2C6Se12 (a) and Mn2C6S6Se6 (b) monolayers from the AIMD simulations at 800 K for 10 ps, and the final structures after the AIMD simulations for Mn2C6Se12 (c) and Mn2C6S6Se6 (d) monolayers.
Figure S2. Spin-dependent band structures for Mn$_2$C$_6$Se$_{12}$ (a) and Mn$_2$C$_6$S$_6$Se$_6$ (b) monolayers within the HSE06 functional.

Figure S3. The orbital-resolved spin-down band structure for the Mn$_2$C$_6$Se$_{12}$ monolayer. The band structures contributed from each atoms (a), the p$_x$, p$_y$ and p$_z$ orbitals of C (b) and Se (c) atoms resolved to the spin down-band, the Mn 5d-derived orbitals to the spin-down band (d). The color intensity represents the amplitude of the P/d-orbital character. The Fermi level is denoted by a dashed line.
**Figure S4.** The schematic for the spintronic device model based on the Mn$_2$C$_6$Se$_{12}$ monolayer.

**Figure S5.** The spin-dependent band structures of the left (a) and right (b) electrodes of Mn$_2$C$_6$Se$_{12}$ monolayer in the parallel configuration of magnetization.

**Figure S6.** The spin-resolved current-voltage curves (a) for the parallel configuration (PC) and the antiparallel configuration (APC) of the device based on the Mn$_2$C$_6$Se$_{12}$ monolayer. The magnetoresistance ratio (MR) (b) versus the bias voltage.