

Supplementary Information

## Modifying spin current filtering and magnetoresistance in a molecular spintronic device

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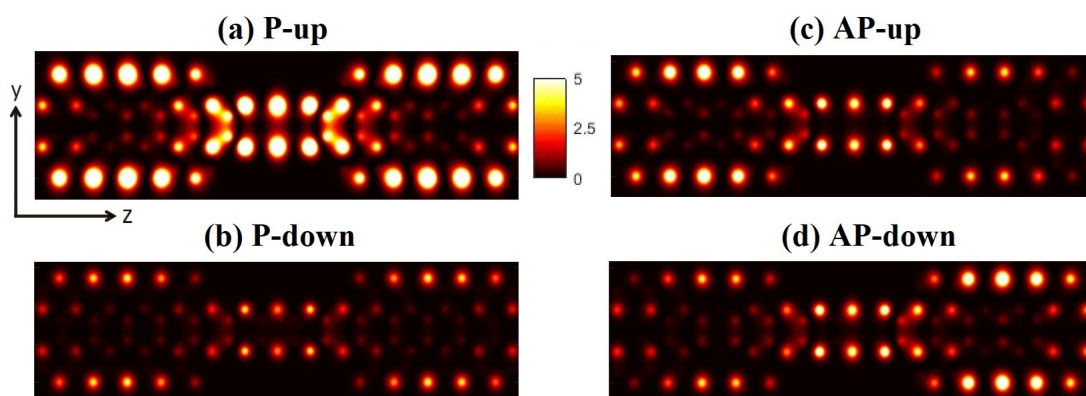


Fig.S1 Local density of states (LDOS) of DDQP device with 4-ZGNR electrodes, for (a) up spin, and (b) down spin electrons of parallel (P) configuration. Panels (c) and (d) are up and down spin electrons LDOS of anti-parallel (AP) configuration, respectively.

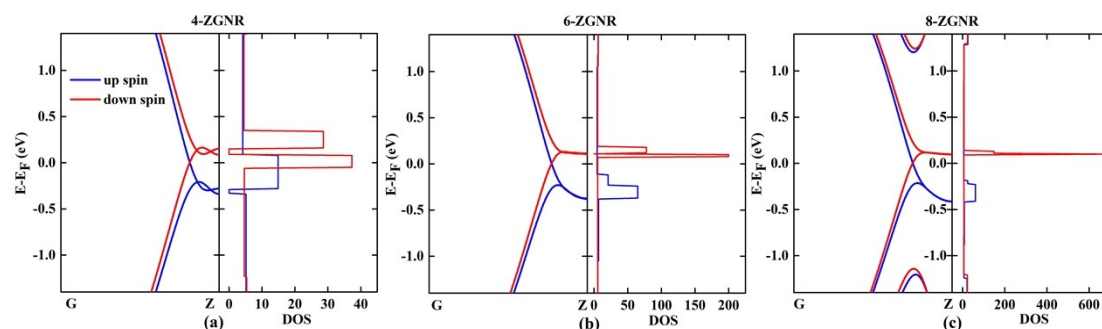


Fig.S2 Band structures and density of states of 4/6/8-ZGNR with two edges of parallel spin moments.

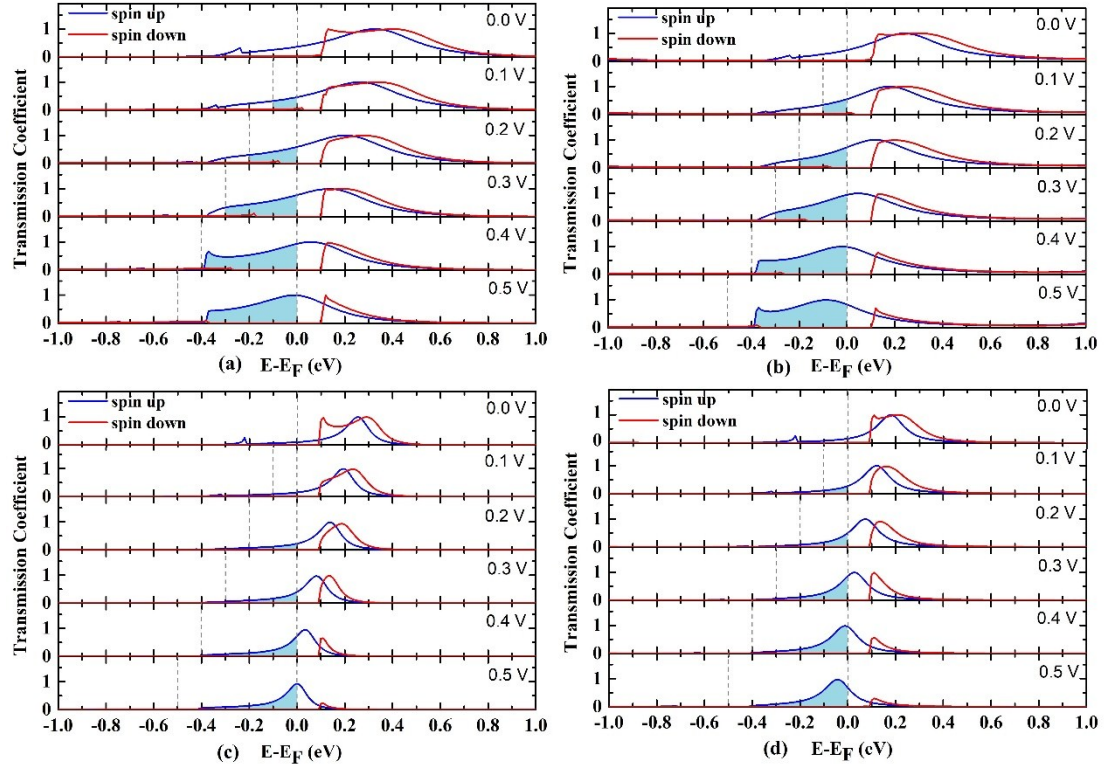


Fig.S3 Transmission spectra of the above-mentioned structures with parallel spin configuration for the structures (a) 6D1, (b) 6D2, (c) 8D1, (d) 8D2. The dashed lines indicate the bias windows.

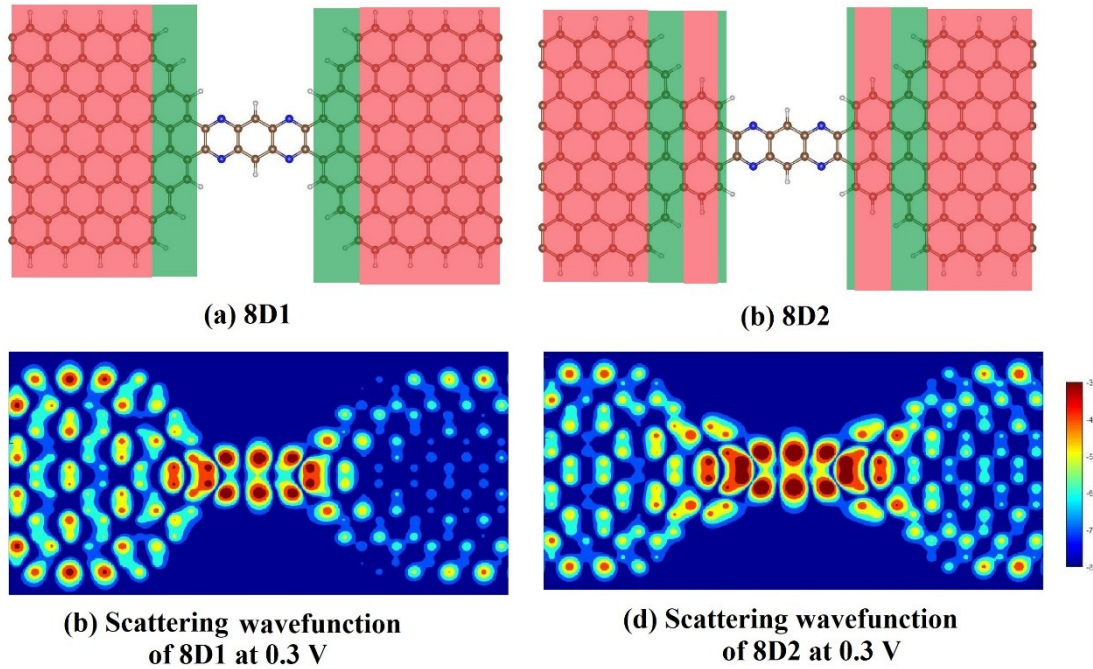


Fig.S4 For (a) 8D1 and (c) 8D2 configurations, in red blocks electrons mainly transport along the zigzag edges, but in green blocks, electrons encounter different transport direction edges with respect to their momentum. (c) and (d) show the scattering wavefunctions of 8D1 and 8D2 under 0.3 bias voltage, respectively.

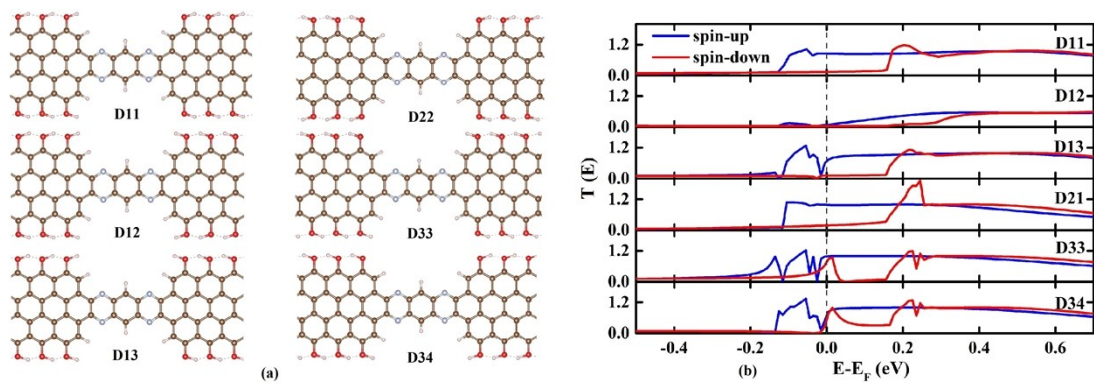


Fig.S5 (a) Schematic illustrations of molecular junctions with hydroxylated ZGNR electrodes; (b) Spin-resolved transmission spectra of the structures under zero bias voltage. At Fermi energy, D11 and D21 shows good separation of different spin, while D33 and D34 are nearly spin degenerate.

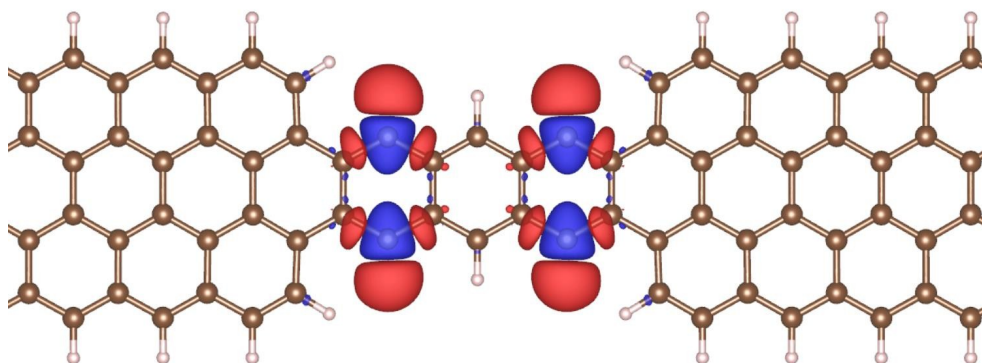


Fig.S6 Differential charge density of the DDQP device versus a 3-Acene device. Blue and red colors correspond to positive and negative differential charge densities, respectively. The calculation was performed using VASP with periodic boundaries, the isosurface level value is set to be 0.056 e/bohr<sup>3</sup>.