Supplementary Material

Perylene-based molecular device: Multifunctional spintronic and spin caloritronic applications

Xuming Wu,[a,b] Shifa Xiao,[a] Jun Quan,[a] Chunhua Tian*[a] and Guoying Gao*[b]

[a]College of Physical Science and Technology, Lingnan Normal University, 524048 Zhanjiang, China. E-mail: chunhuatian@lingnan.edu.cn

[b]School of Physics and Wuhan National High Magnetic Field Center, Huazhong University of Science and Technology, Wuhan 430074, China. E-mail: guoying_gao@mail.hust.edu.cn

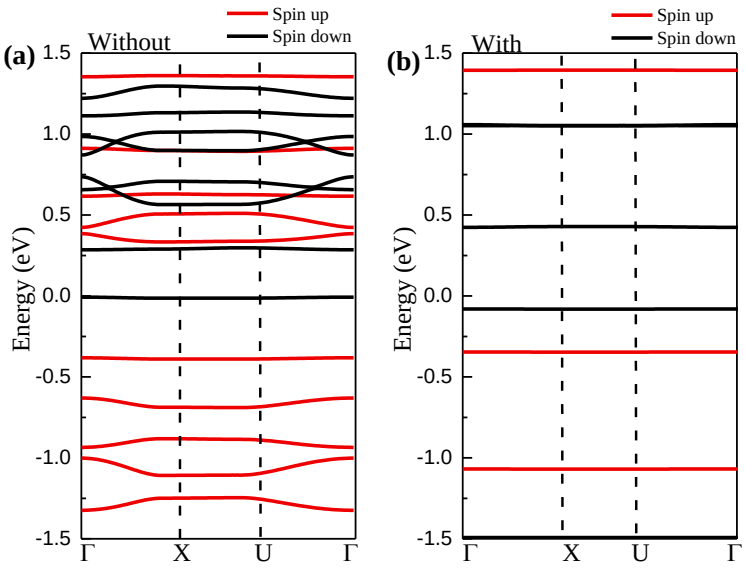

Fig. S1 The spin-dependent band structure of the perylene molecule without (a) and with (b) hydrogenation.

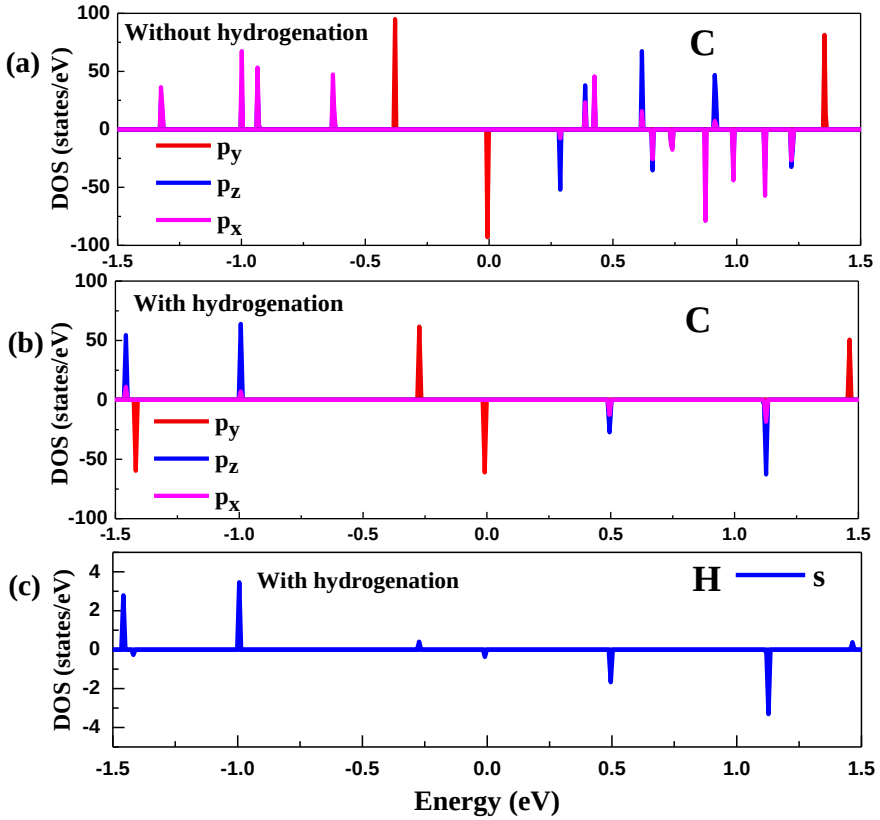

Fig. S2 The spin-dependent main atomic orbital density of states of the perylene molecule without (a) and with (b,c) hydrogenation.

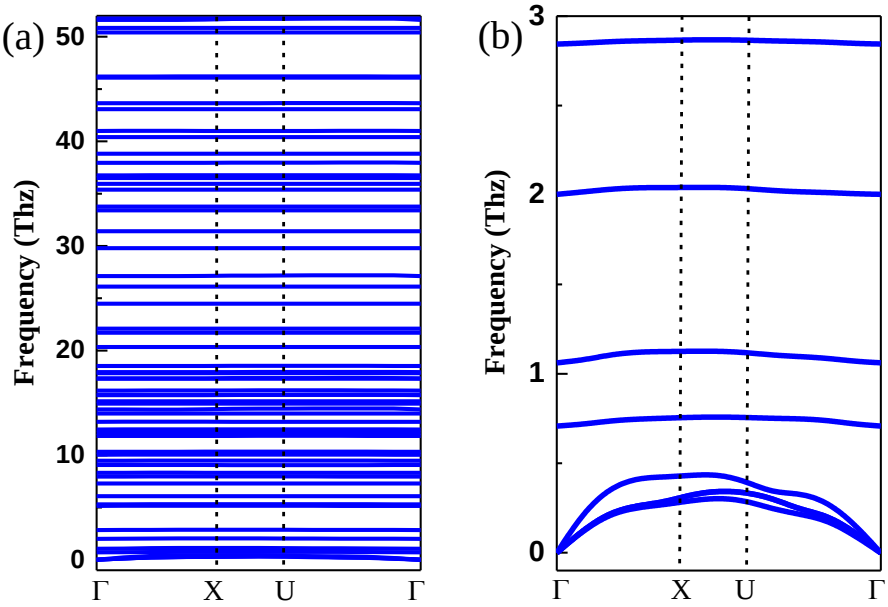

Fig. S3 The phonon spectrum of the perylene molecule, which is presented in a smaller frequency range (b) in order to indicate whether there is imaginary frequency.

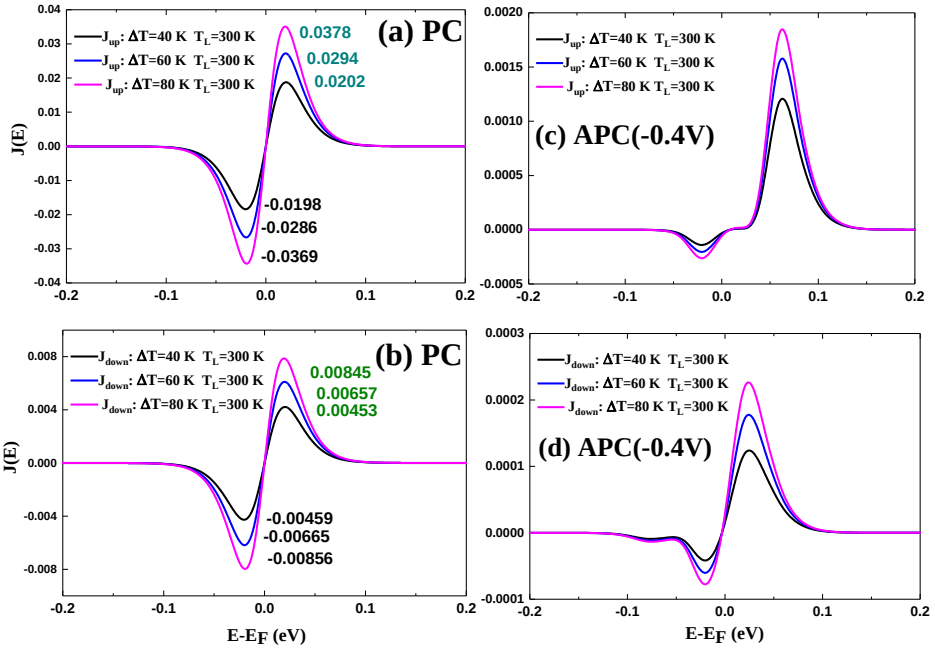

Fig. S4 The spin-up (a) and spin-down (b) Fermi-Dirac distribution differences at ΔT = 40, 60 and 80 K as a function of energy in PC at T_L =300 K, (c) and (d) are the same as (a) and (b) but in APC.

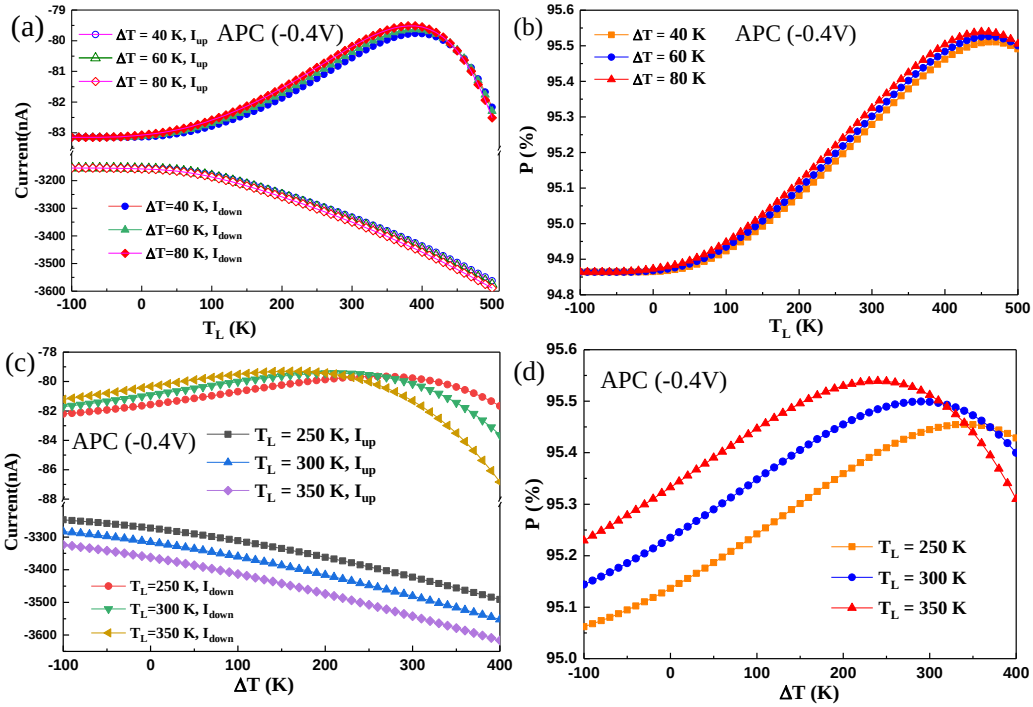

Fig. S5 The thermal spin-dependent current versus T_L for different ΔT (a) and versus ΔT for different T_L (c) in APC at the bias voltage of -0.4 V. The corresponding polarization of thermal spin current versus T_L for different ΔT (b) and versus ΔT for different T_L (d).