

Supporting Information

Electrical tuning of spin current in a boron nitride nanotube quantum dot

Kamal B Dhungana¹ and Ranjit Pati*¹

¹*Department of Physics, Michigan Technological University, Houghton MI 49931, USA*

* e-mail: patir@mtu.edu

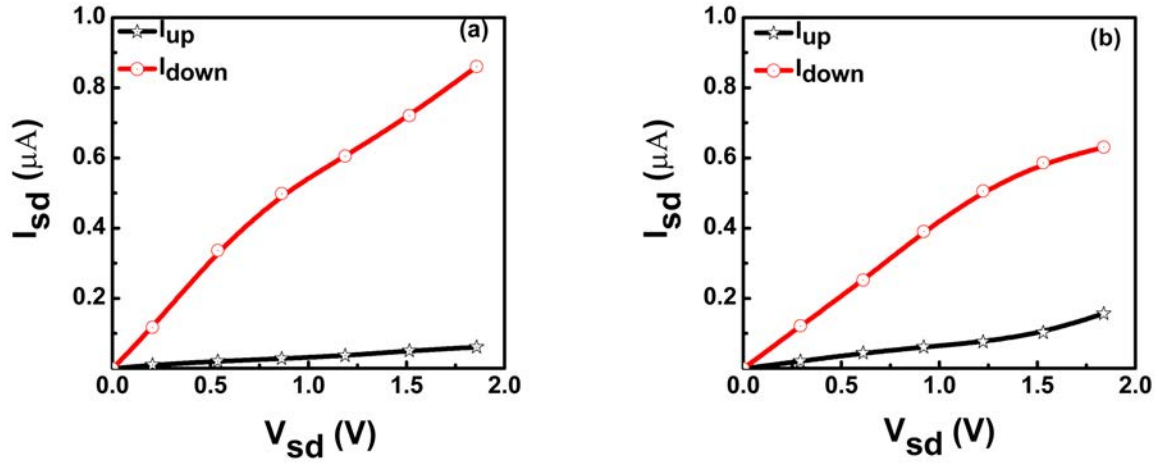


FIG. 1: **Spin polarized current.** Bias dependent spin-up (I_{up}) and spin-down (I_{down}) component of the current at $\varepsilon_g = 0$ V/Å; spin-down contribution to current is higher in both (a) Parallel Spin Configuration (PC) and (b) Anti-parallel Spin Configuration (APC).

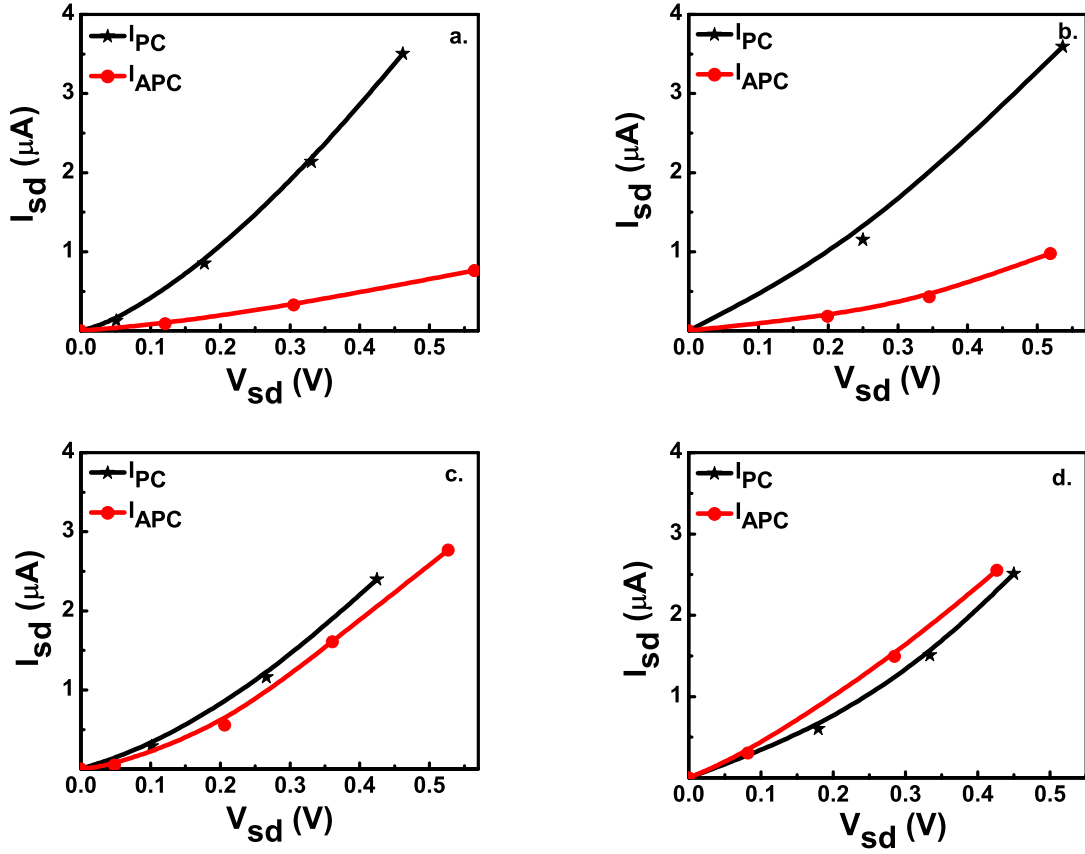


FIG. 2: **Spin dependent current in (7,0) BNTQD tunnel junction.** I_{sd} - V_{sd} curves for parallel (PC) and anti-parallel (APC) spin configuration for different transverse electric fields: (a) $\varepsilon_g = 0.0 \text{ V/\AA}$, (b) $\varepsilon_g = 0.41 \text{ V/\AA}$, (c) $\varepsilon_g = 0.61 \text{ V/\AA}$, (d) $\varepsilon_g = 0.81 \text{ V/\AA}$. In the case of PC, current decreases with the increase of ε_g , whereas in the case of APC, the current increases with the increase of ε_g as observed in the (6,0) BNTQD tunnel junction. It can be clearly seen from figure (d) that the I_{APC} exceeds I_{PC} resulting in a switching in the sign of TMR from positive to negative as seen from Fig. 1c for the (6,0) BNTQD tunnel junction.

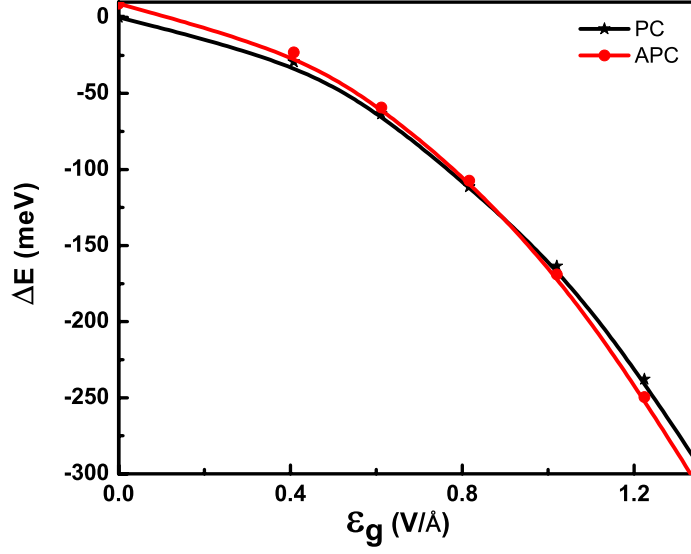


FIG. 3: **Sign reversal of exchange energy in (7,0) BNTQD tunnel junction.** $\Delta E_{PC/APC}(\epsilon_g) = E_{PC/APC}(\epsilon_g) - E_{PC}(\epsilon_g = 0)$; E_{PC} and E_{APC} correspond to the energy for the PC and APC, respectively. $E_{PC}(\epsilon_g = 0)$ is the reference energy. The crossing of ΔE for PC and APC confirms the sign change in exchange coupling as observed for the (6, 0) BNTQD tunnel junction.

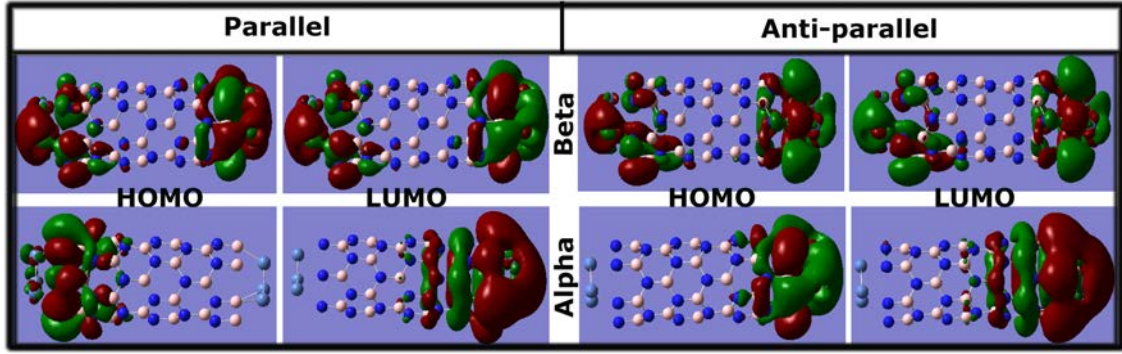


FIG. 4: **Frontier molecular spin-orbitals.** Highest occupied molecular orbital (HOMO) and Lowest Unoccupied molecular orbital (LUMO) for the spin up (Alpha) and spin down (Beta) states of the extended BNTQD-Ni system at $\varepsilon_g = 0 \text{ V/\AA}$. For both parallel (PC) and anti-parallel (APC) spin configurations between the electrodes, the electron cloud is distributed at both interfaces for the spin down state. This explains the observed higher current contribution from the Beta state. A detailed analysis of the orbitals of the Beta state for the PC and APC show that B and N atoms at the two opposite interfaces have primarily s and p orbital characters whereas the Nickel has mostly s and d characters. In the case of Alpha state, for the PC, HOMO has N(s, p) and very small Ni(s), whereas the LUMO has B (s, p) and Ni(s, d) at one interface with s-being the dominant orbital character. For the APC in the Alpha state, HOMO has B(s, p) and Ni (s, d) characters; LUMO has B(s, p) and Ni(s, d) with s-being the dominant character.