

## Supporting Information

# Fullerene-based Single Molecule Diodes with Huge Rectification Ratios: A DFT-NEGF Study

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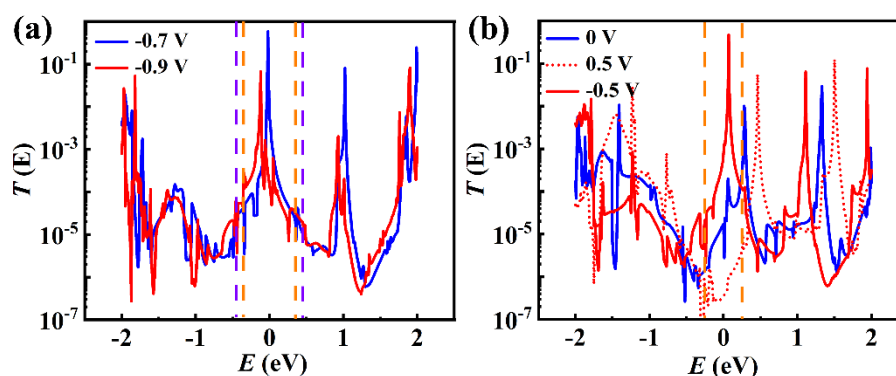


Figure S1. Transmission spectra of the S-DPA-N-C<sub>60</sub> device under the bias of (a) -0.7 V, -0.9 V and (b) 0 V, ±0.5 V. The purple/yellow dashed lines are the boundaries of the bias windows.

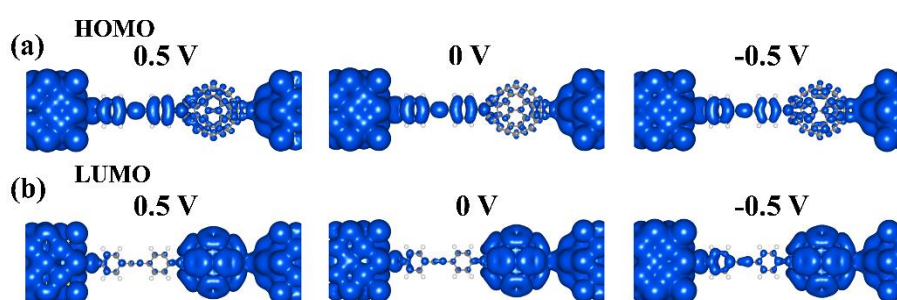


Figure S2. Real space local density of states of (a) HOMO and (b) LUMO orbitals of the S-DPA-N-C<sub>60</sub> device under  $V_b = 0$  V, ±0.5 V.

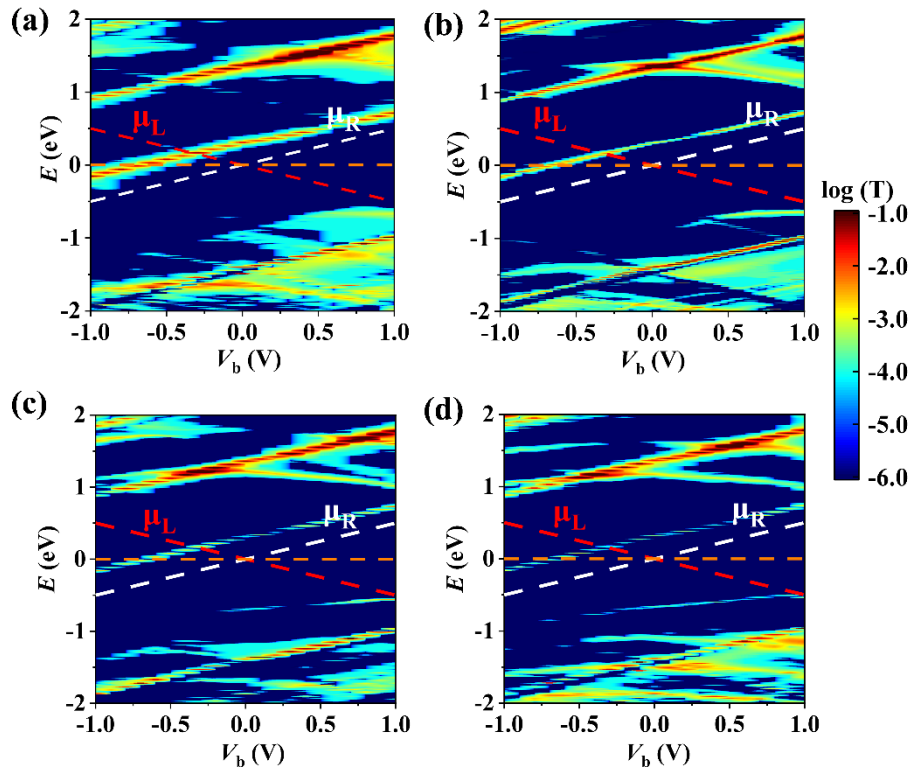


Figure S3. Transmission spectra ( $T(E, V_b)$ ) of S-C<sub>6</sub>H<sub>4</sub>-(C≡C-C<sub>6</sub>H<sub>4</sub>)<sub>*n*</sub>-N-C<sub>60</sub> devices with different lengths (a)  $n = 2$  (b)  $n = 3$  (c)  $n = 4$  and (d)  $n = 5$  under bias  $V_b \in [-1, 1]$  V.

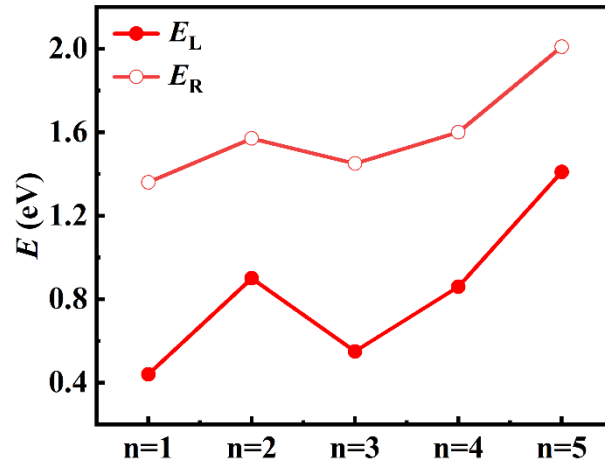


Figure S4. Variation of interactions at the interfaces between the molecule and buffer layers with the length of the molecule for S-C<sub>6</sub>H<sub>4</sub>-(C≡C-C<sub>6</sub>H<sub>4</sub>)<sub>*n*</sub>-N-C<sub>60</sub> devices. .

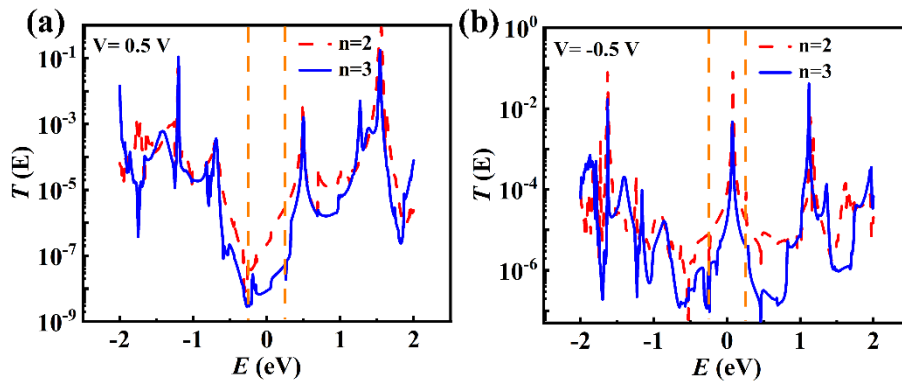


Figure S5. Transmission spectra of  $S-C_6H_4-(C\equiv C-C_6H_4)_n-N-C_{60}$  devices with  $n = 2$  and  $n = 3$  under the bias of (a) 0.5 V and (b) -0.5 V.

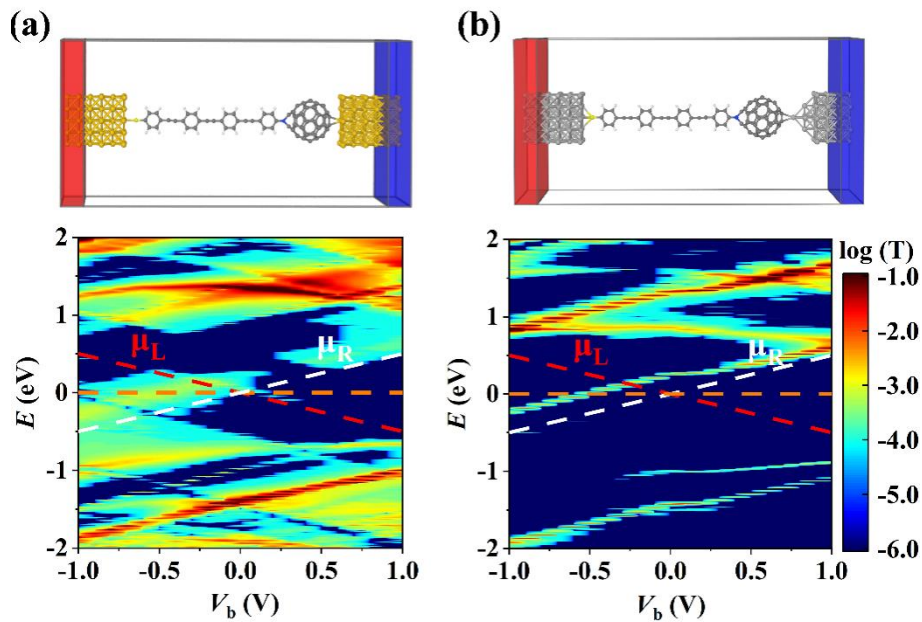


Figure S6. Transmission spectra ( $T(E, V_b)$ ) of  $S-C_6H_4-(C\equiv C-C_6H_4)_3-N-C_{60}$  devices with gold terrace (ter) right electrode ( $Au_{ter}$ ) and silver tip right electrode ( $Ag_{tip}$ ).

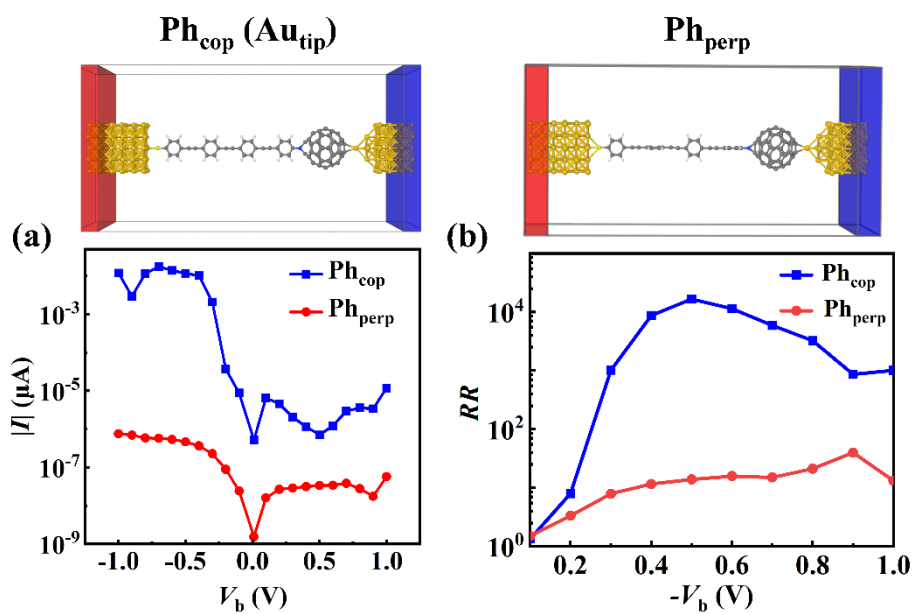


Figure S7. (a) Current-voltage ( $I$ - $V_b$ ) curves and (b) rectification ratio (RR) curves for S-C<sub>6</sub>H<sub>4</sub>-(-C≡C-C<sub>6</sub>H<sub>4</sub>)<sub>3</sub>-N-C<sub>60</sub> device with coplanar (cop) and perpendicular (perp) phenylacetylenes (Ph).