

# SUPPORTING INFORMATION

## Exploring the Odd-Even Effect, Current Stabilization, and Negative Differential Resistance in Carbon Chain-Based Molecular Devices

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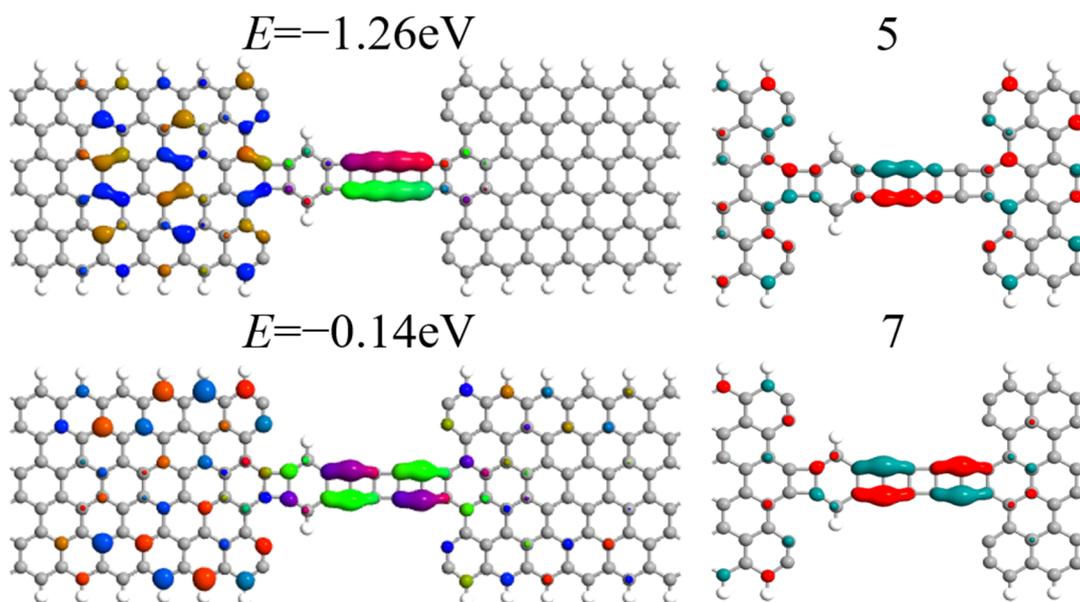


Figure S 1. For D1: The transport modes at  $E = -1.26$ ,  $-0.14$  eV and the wave functions for  $k=0$  states in bands 5 and 7 are presented correspondingly.

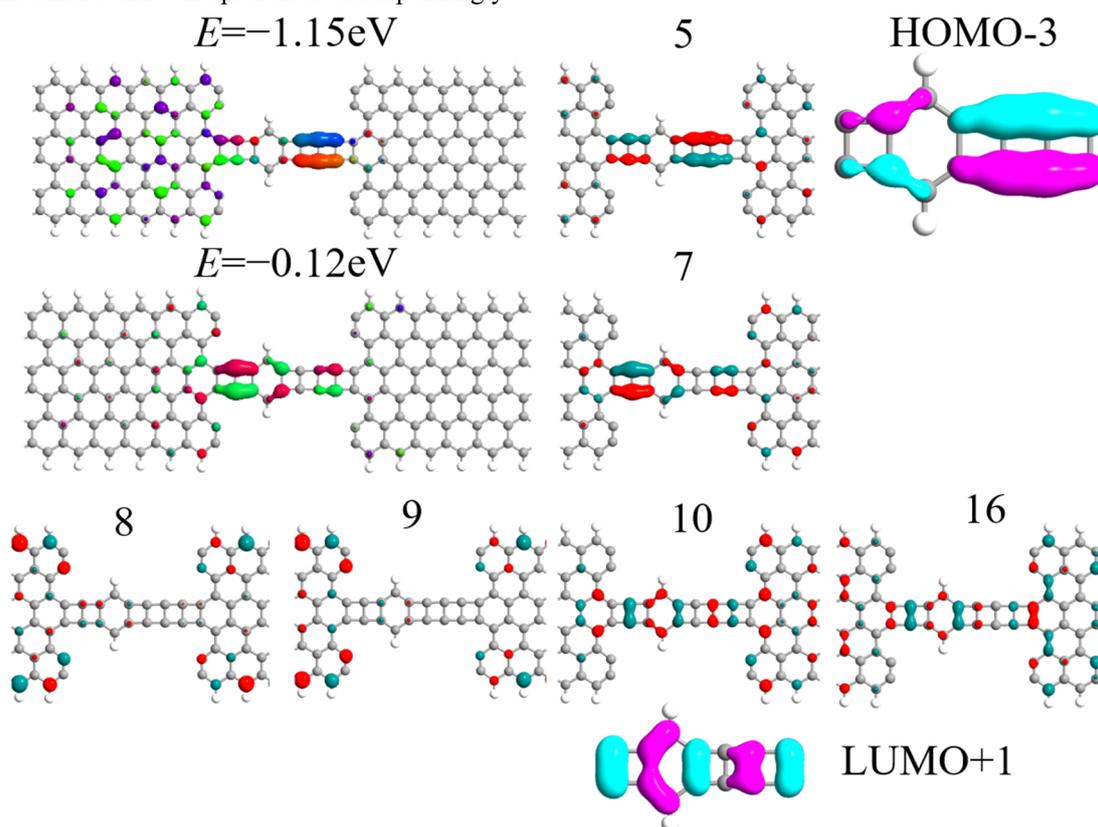


Figure S 2. For D2: The transport modes at  $E = -1.15$ ,  $-0.12\text{eV}$ ; the wave functions for  $k=0$  states in bands 5, 7, 8, 9, 10 and 16; the wave functions of LUMO+1 and HOMO-3 of central molecule.

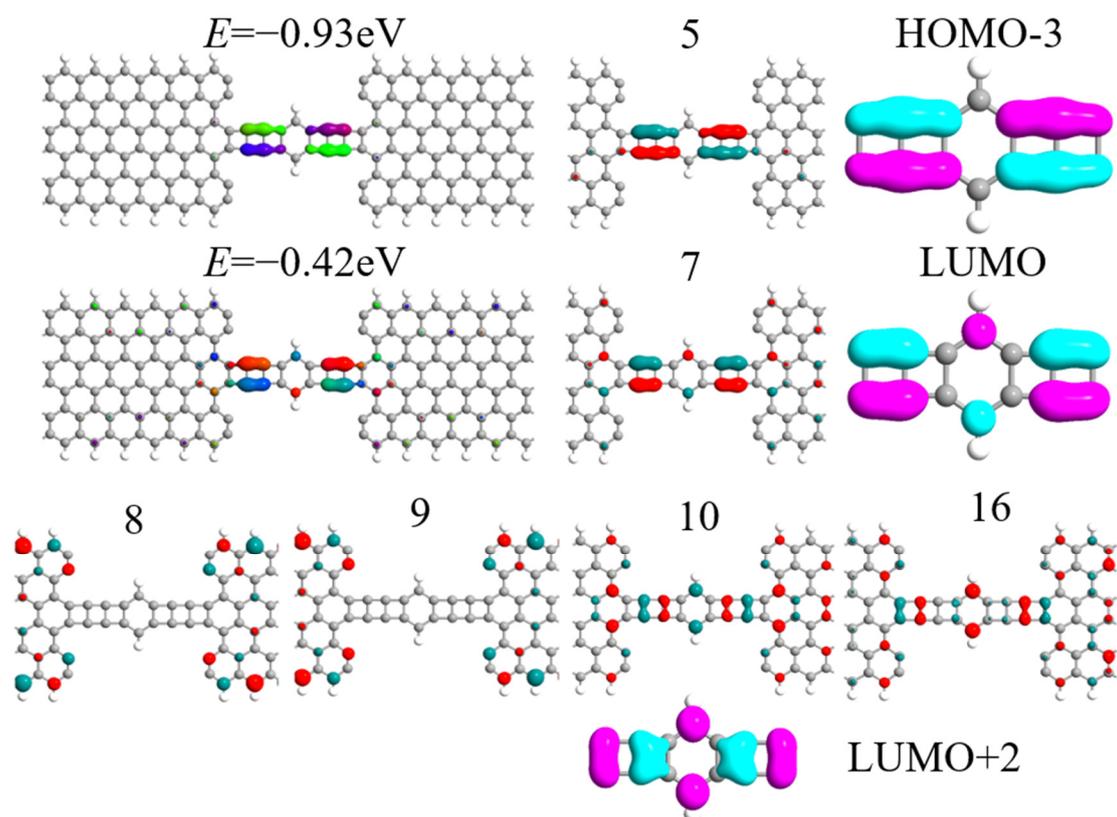


Figure S 3. For D3: The transport modes at  $E = -0.93, -0.42 \text{ eV}$ ; the wave functions for  $k=0$  states in bands 5, 7, 8, 9, 10 and 16; the wave functions of LUMO+2, LUMO and HOMO-3 of central molecule.

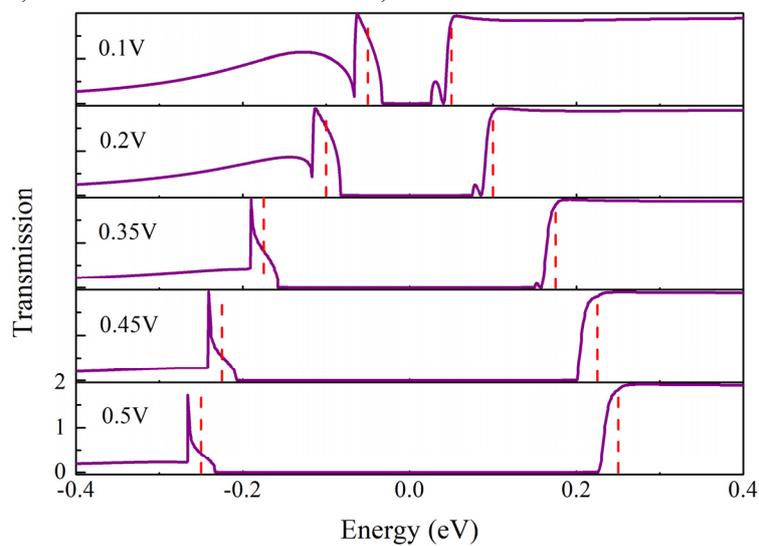


Figure S 4. Transmission spectra of D1 at different bias voltage.

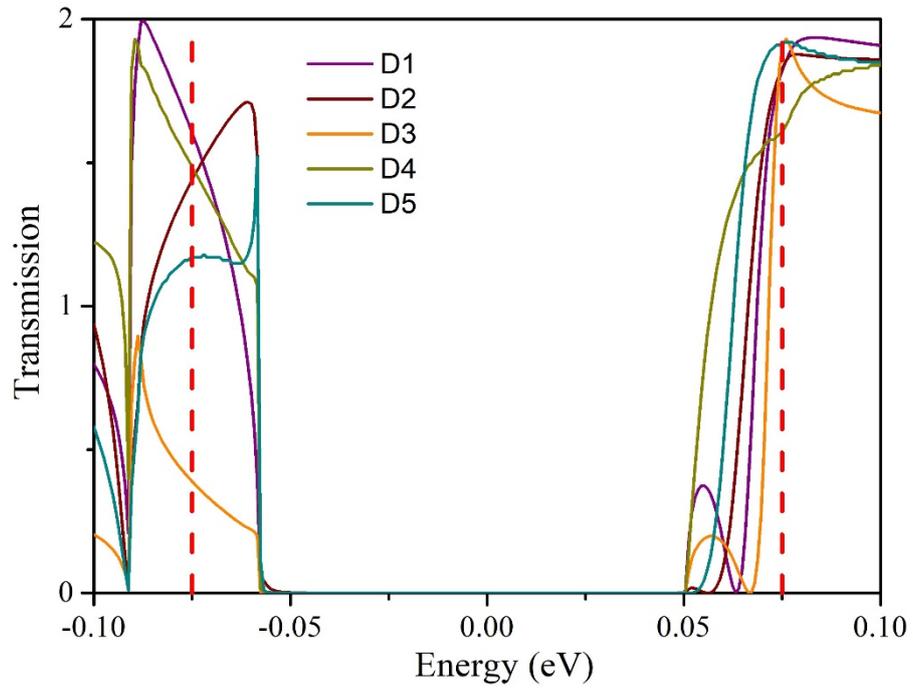


Figure S 5. 0.15V-bias-transmission spectra of D1–D5.