

NDR and spin-polarized transport properties of magnetic Fe sandwiched C₆₀-GNR single molecule devices: theoretical insight

Xiaohui Liu, Yan Shang,* Yangyang Hu, Zhaodi Yang, Ya Wang, Lei Pei, Hong Yu, Munir Ur Rehman, Yuqi Dong, Lu Han, Guiling Zhang*

School of Materials Science and Engineering, Harbin University of Science and Technology, Harbin, 150080, China. E-mail: shangyan1972@126.com, guiling-002@163.com

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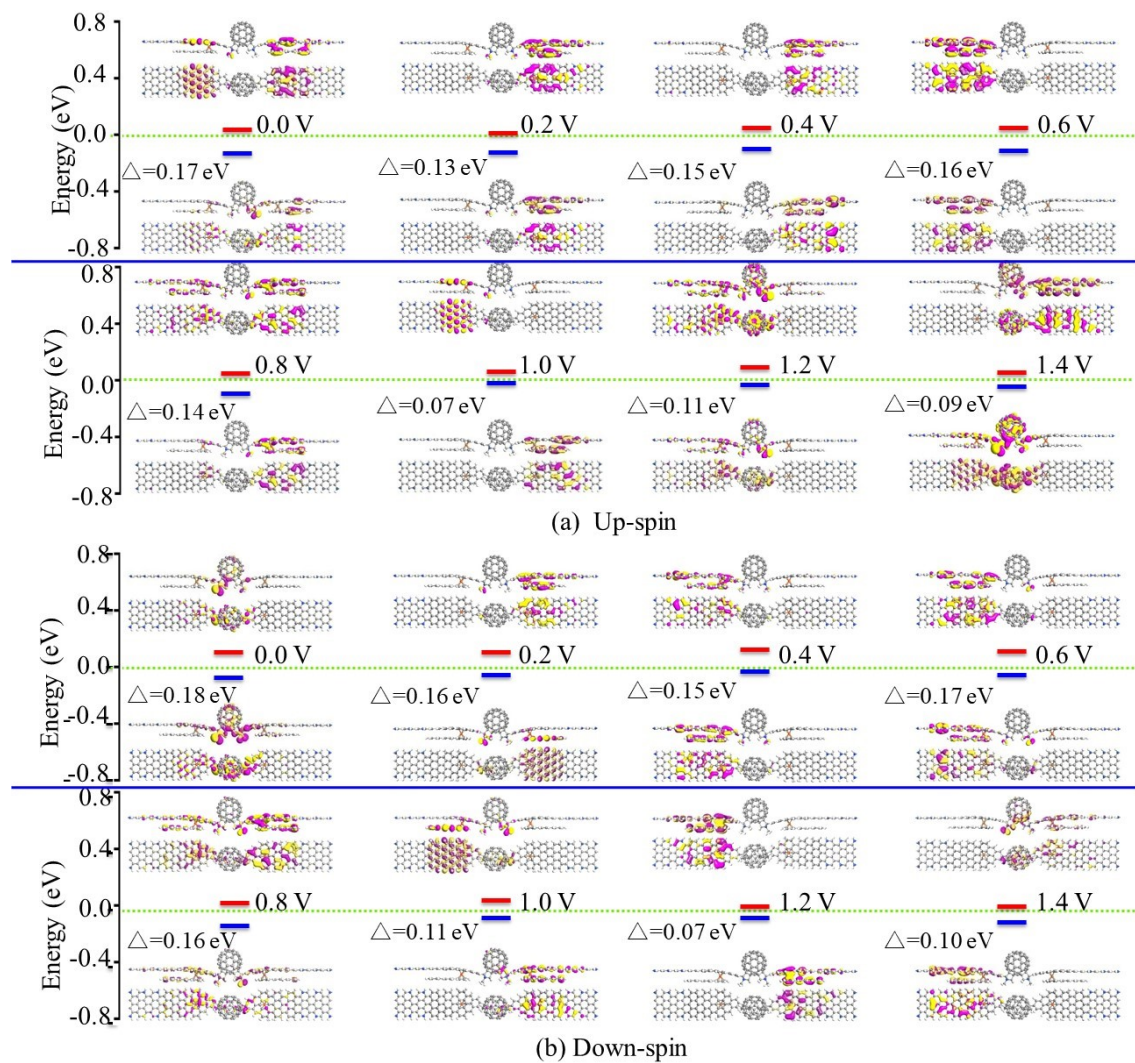


Figure S1 Spin-resolved MPSH HOMO and LUMO of the AIA' device under various bias. (a) and (b) are for up-spin and down spin channels, respectively.

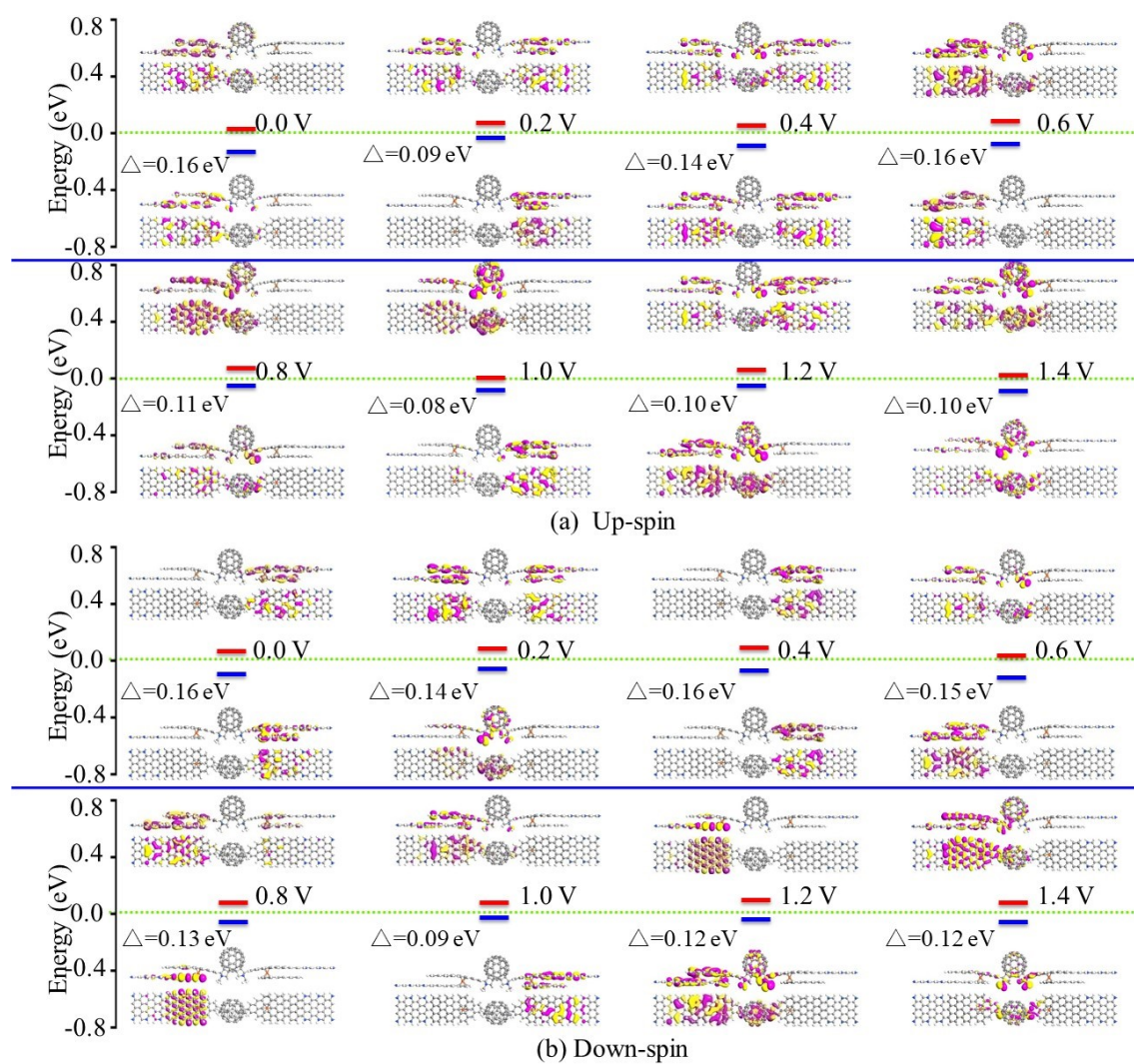


Figure S2 Spin-resolved MPSH HOMO and LUMO of the BIA device under various bias. (a) and (b) are for up-spin and down spin channels, respectively.

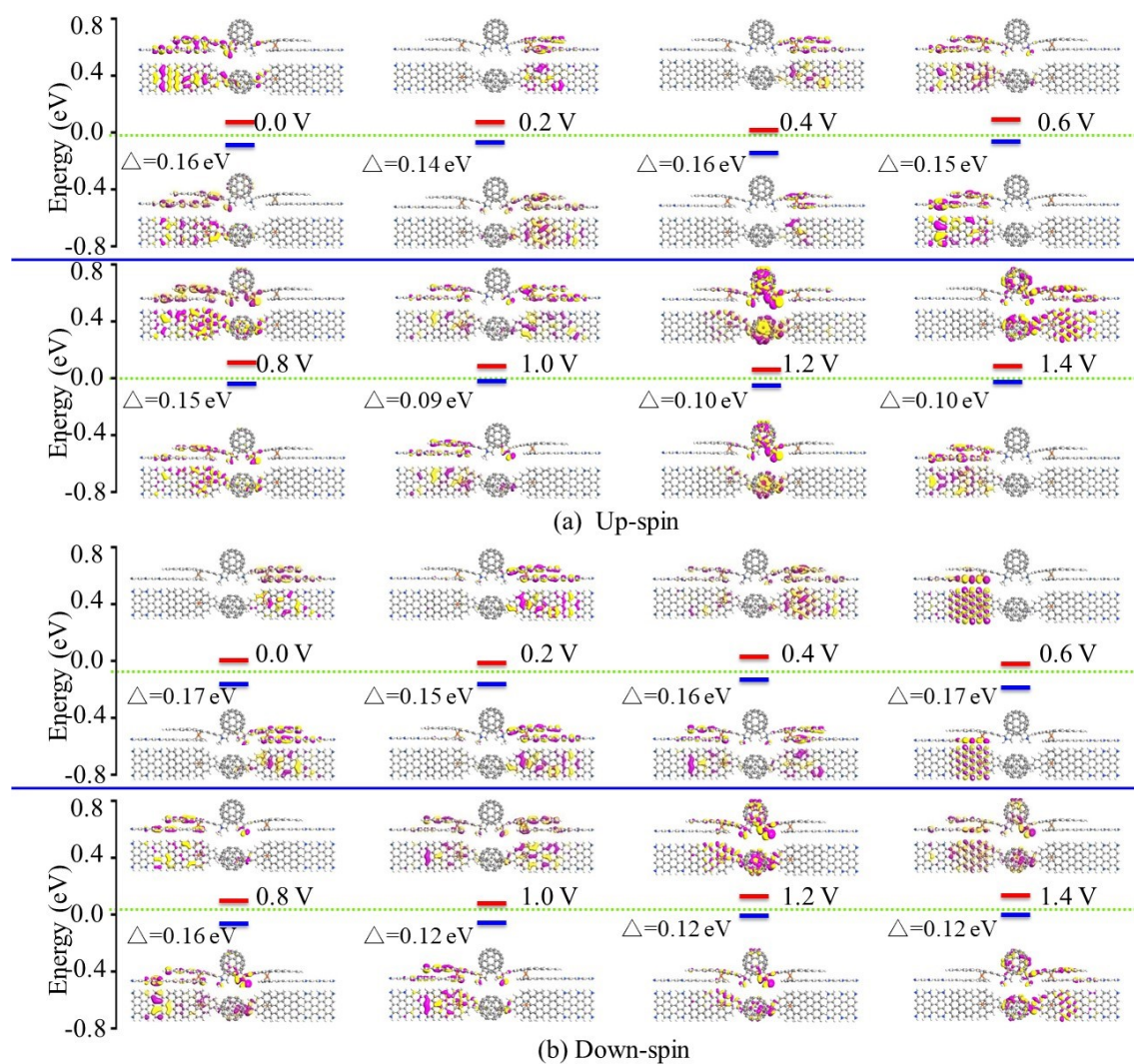


Figure S3 Spin-resolved MPSH HOMO and LUMO of the **BIB'** device under various bias. (a) and (b) are for up-spin and down spin channels, respectively.

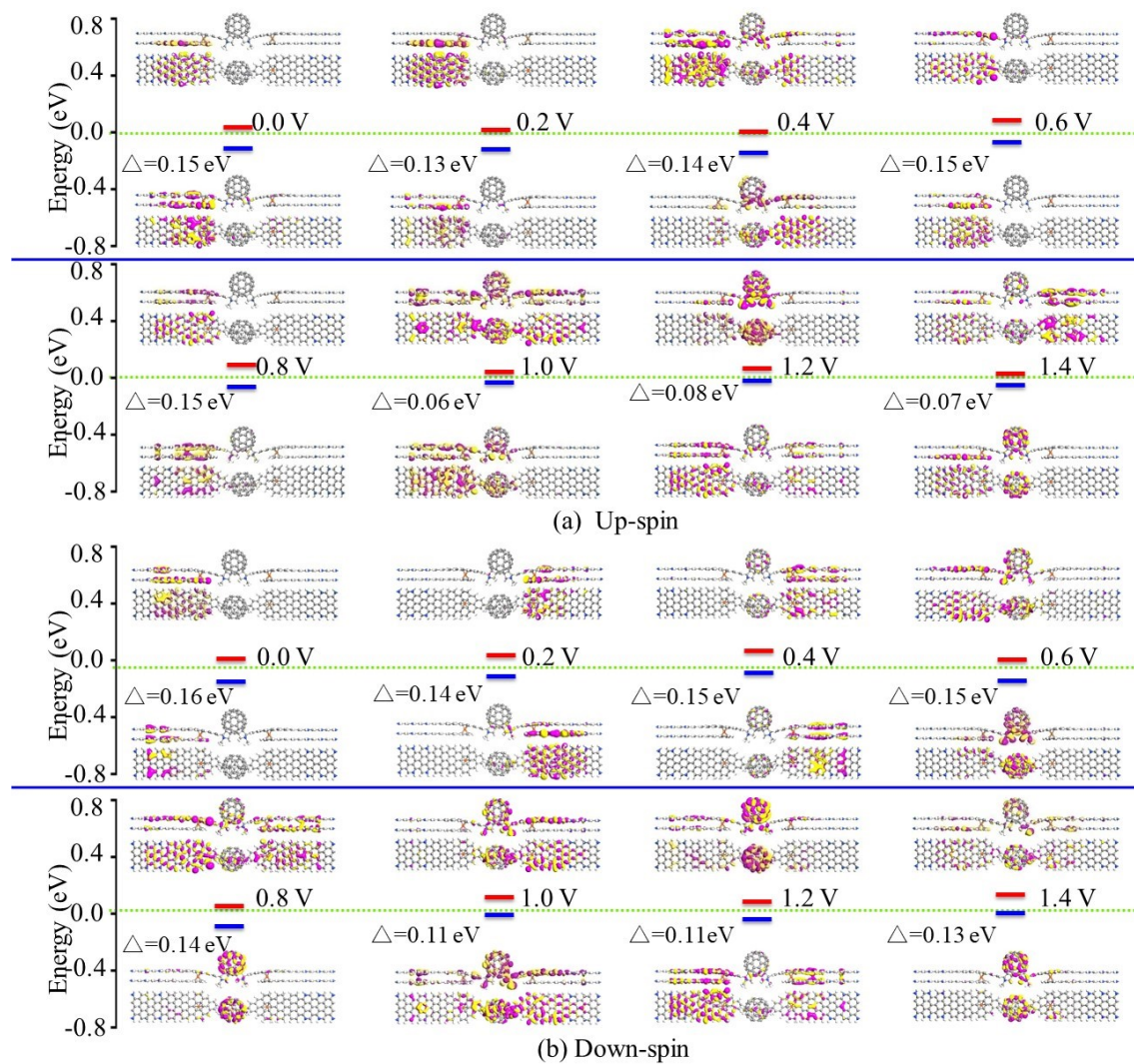


Figure S4 Spin-resolved MPSH HOMO and LUMO of the **ABIA 'B'** device under various bias. (a) and (b) are for up-spin and down spin channels, respectively.

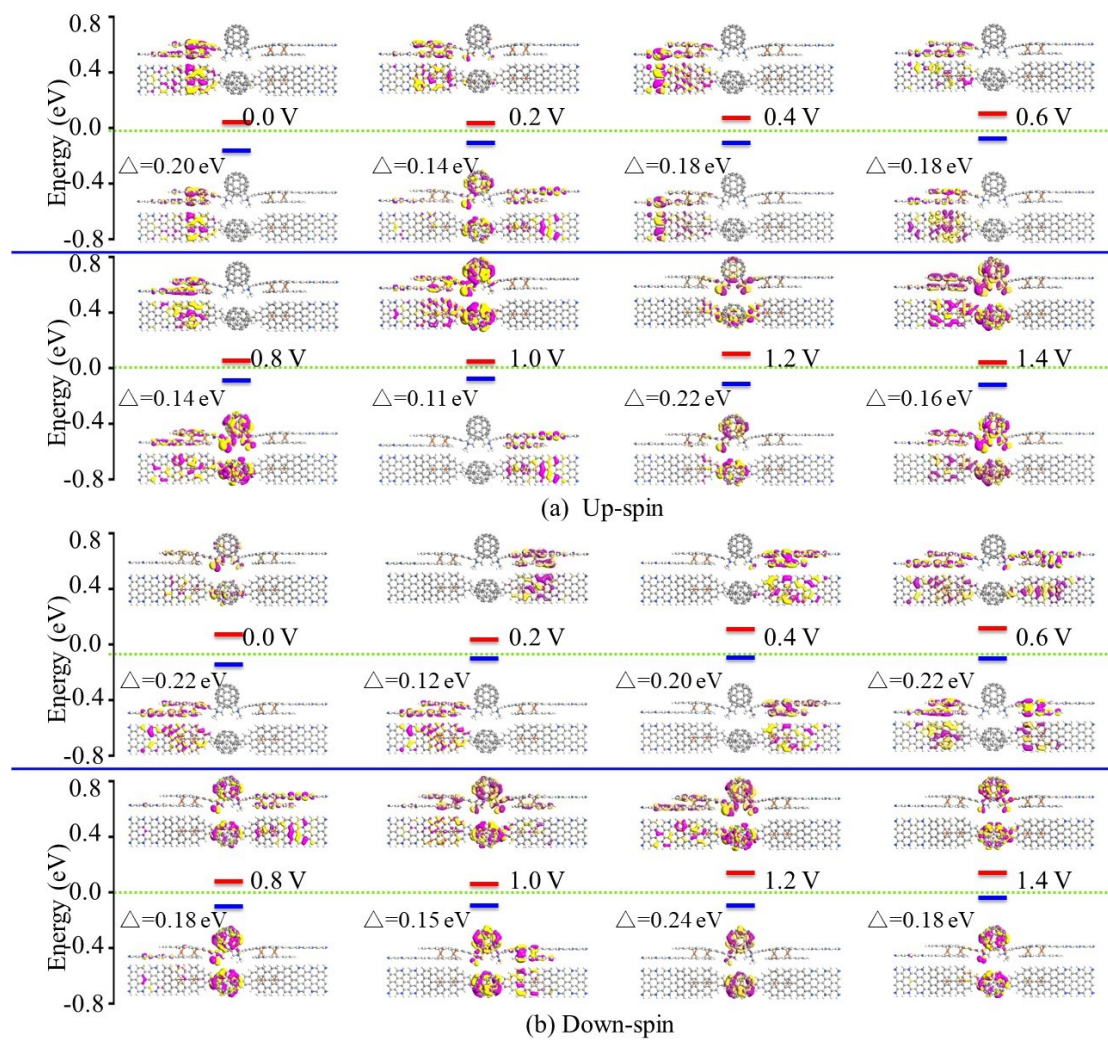


Figure S5 Spin-resolved MPSH HOMO and LUMO of the **BIIA'** device under various bias. (a) and (b) are for up-spin and down spin channels, respectively.

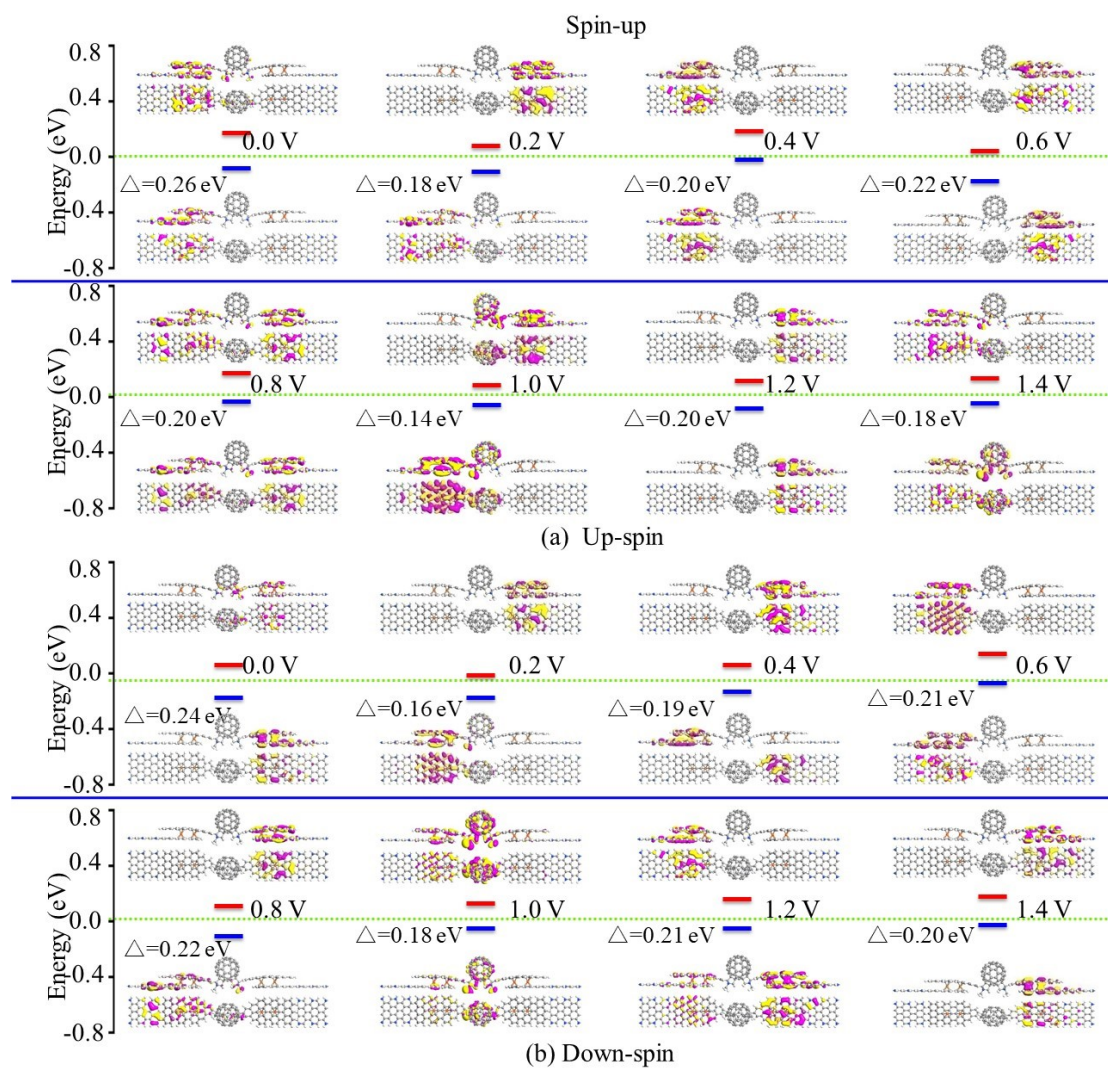


Figure S6 Spin-resolved MPSH HOMO and LUMO of the **BIIB'** device under various bias. (a) and (b) are for up-spin and down spin channels, respectively.

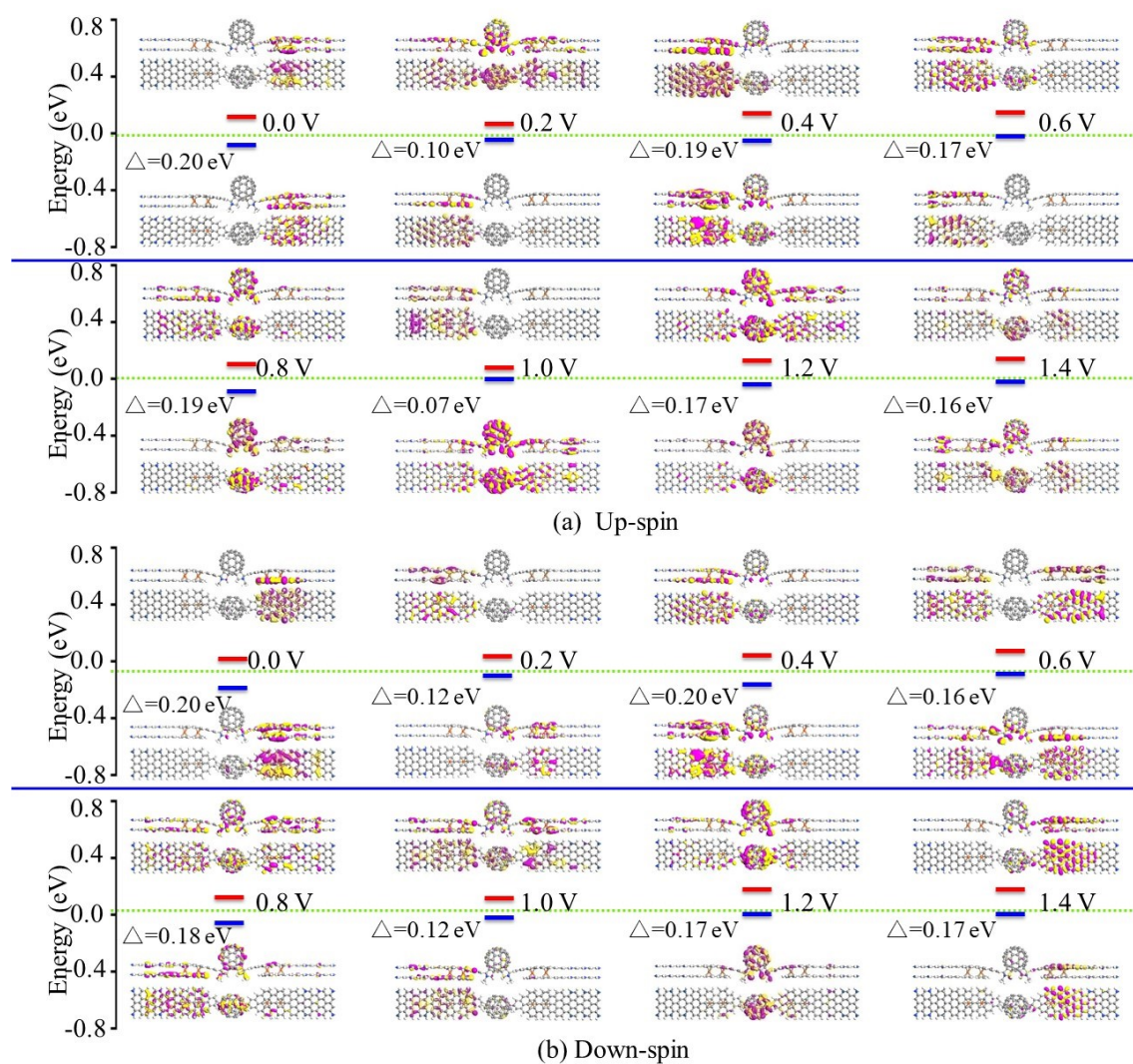


Figure S7 Spin-resolved MPSH HOMO and LUMO of the **ABIIA'B'** device under various bias. (a) and (b) are for up-spin and down spin channels, respectively.

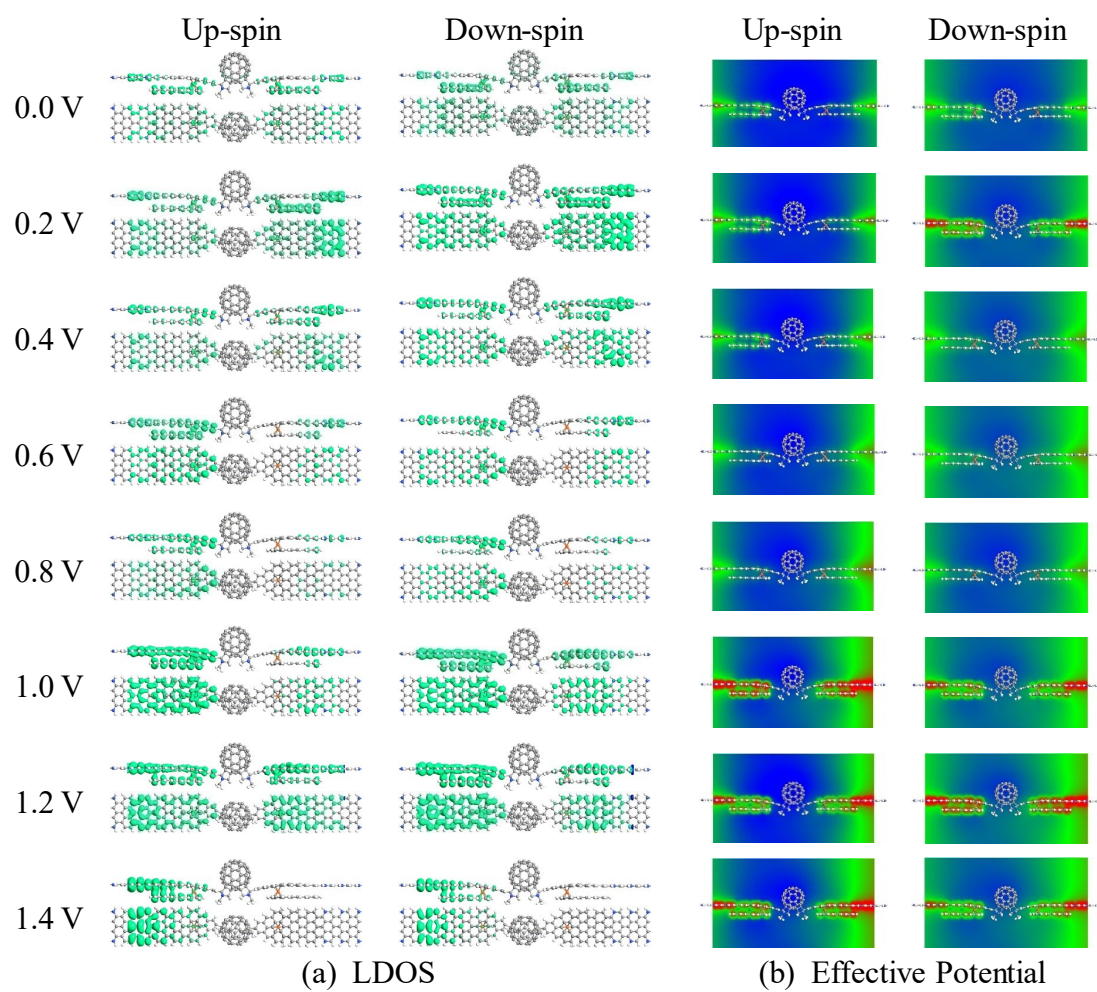


Figure S8 Spin-resolved (a) LDOS and (b) effective potentials of the AIA' device under various biases.

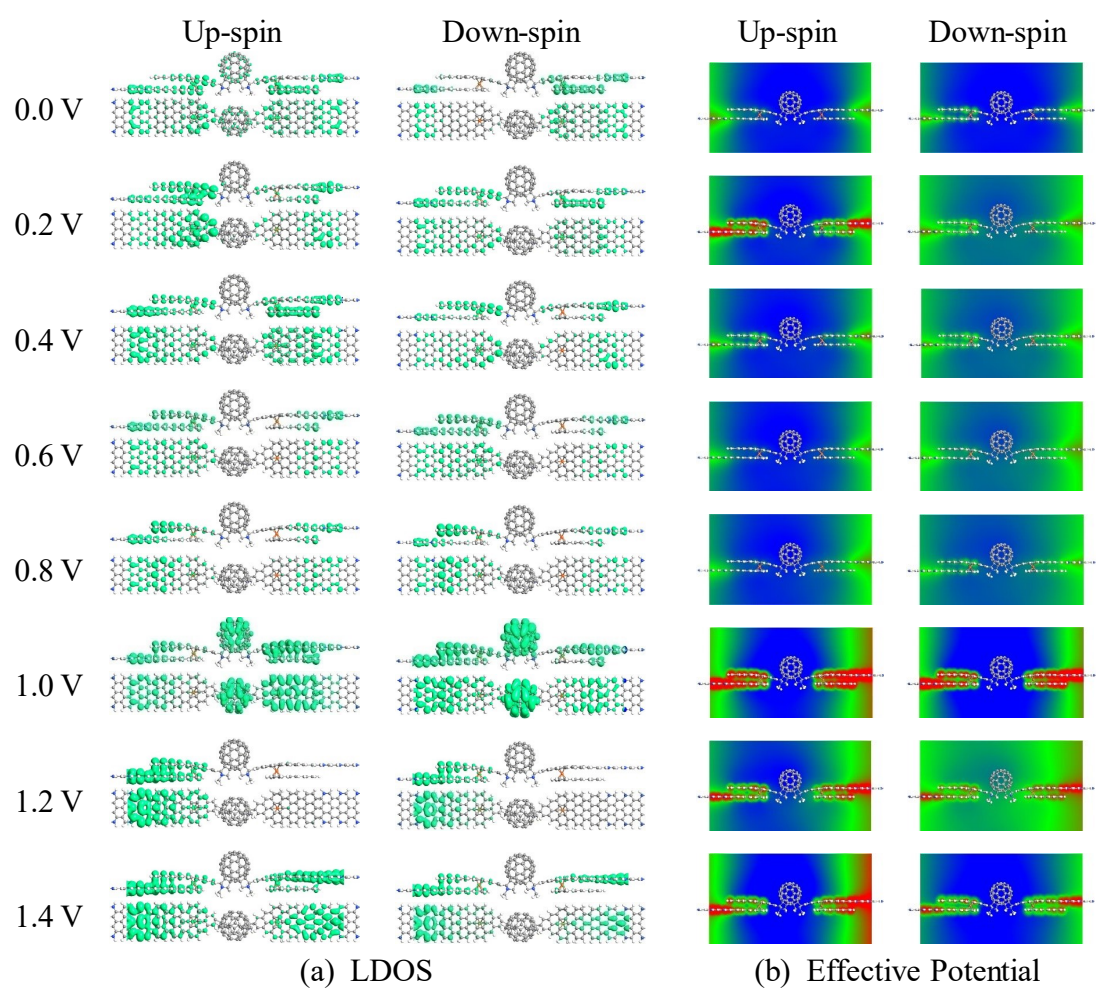


Figure S9 Spin-resolved (a) LDOS and (b) effective potentials of the **BIA'** device under various biases.

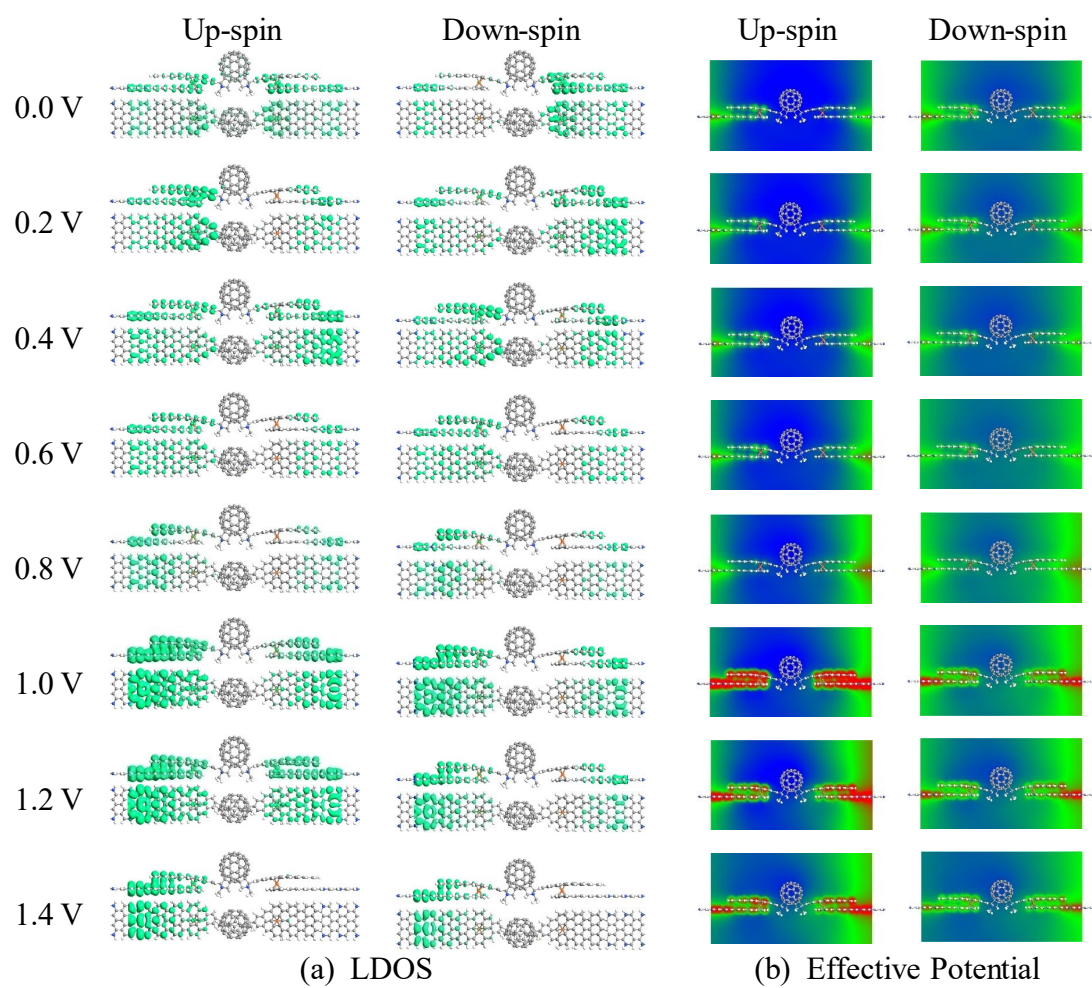


Figure S10 Spin-resolved(a) LDOS and (b) effective potentials of the **BIB'** device under various biases.

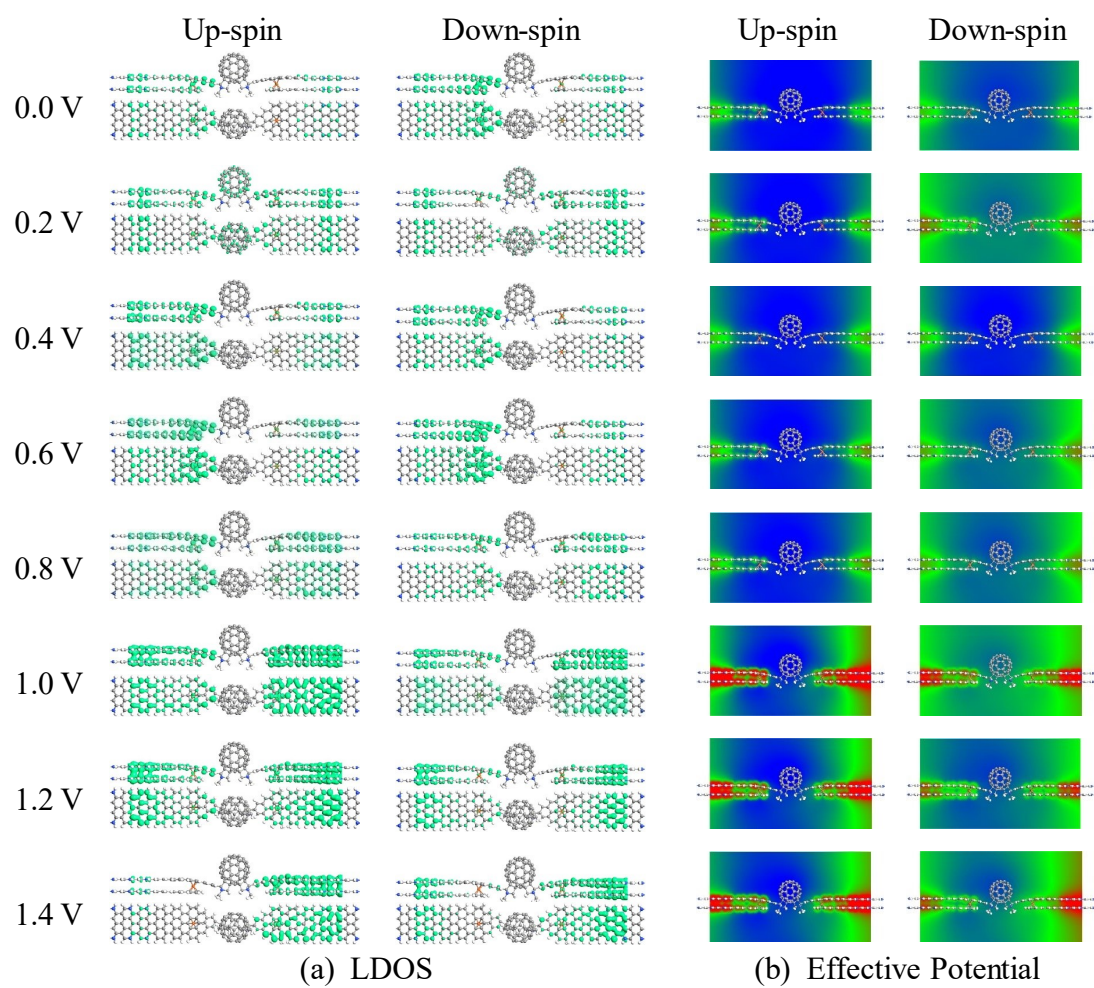


Figure S11 Spin-resolved(a) LDOS and (b) effective potentials of the ABIA'B' device under various biases.

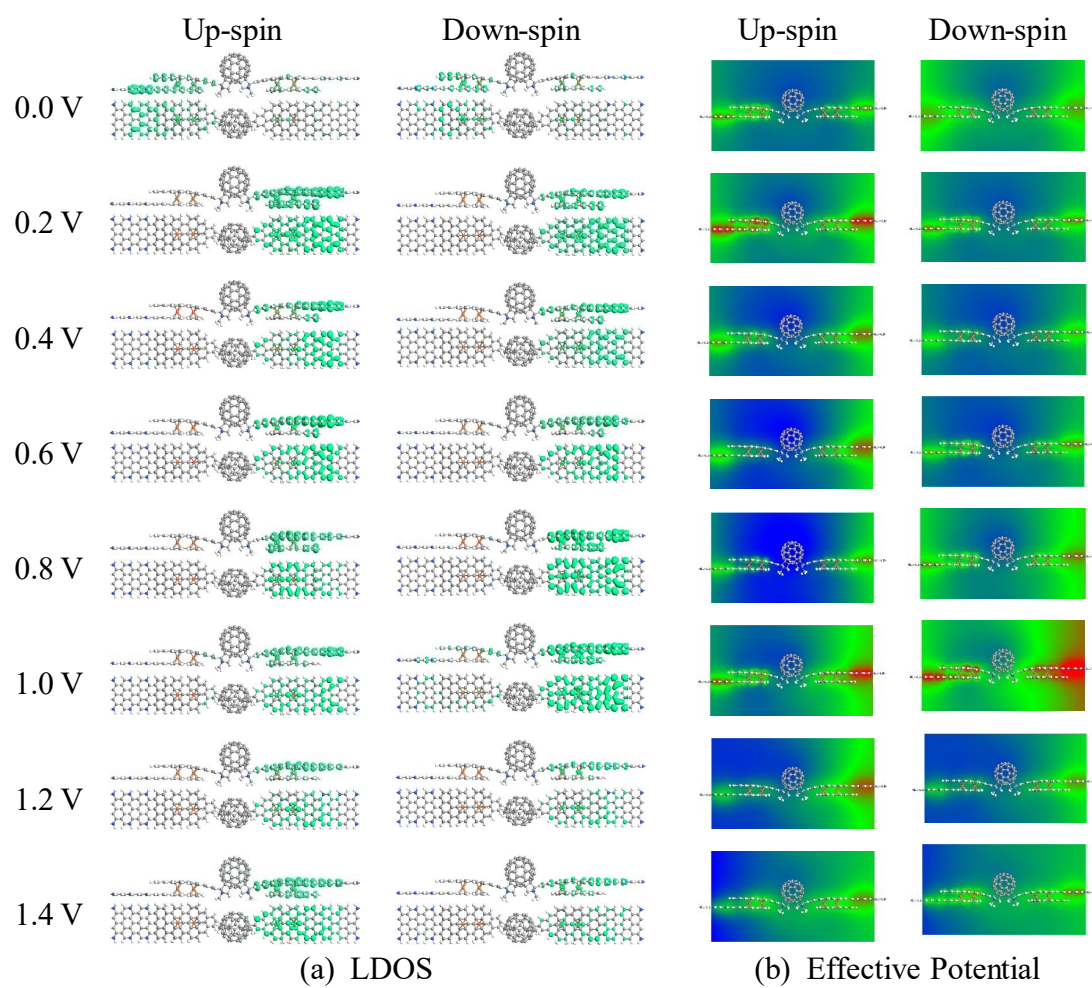


Figure S12 Spin-resolved (a) LDOS and (b) effective potentials of the **BIIA'** device under various biases.

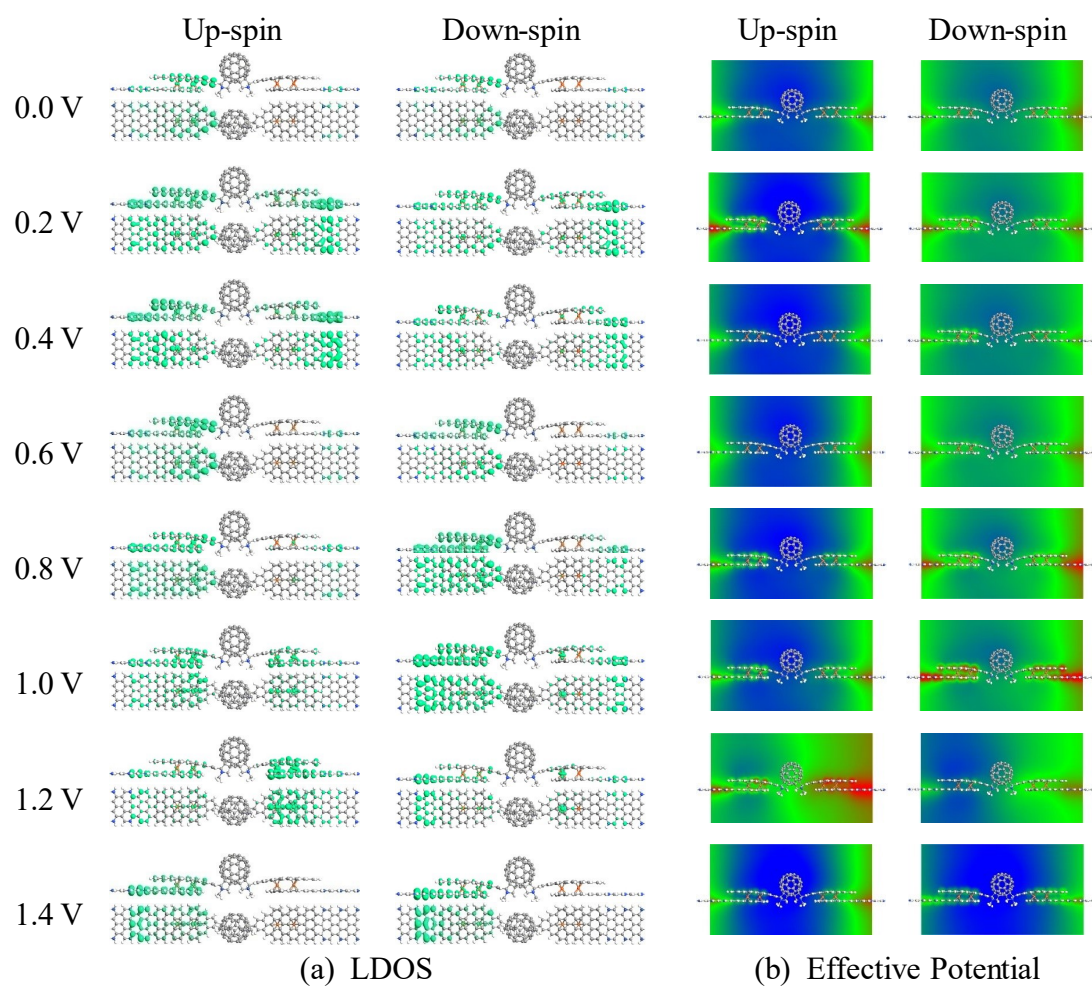


Figure S13 Spin-resolved (a) LDOS and (b) effective potentials of the **BIIB'** device under various biases.

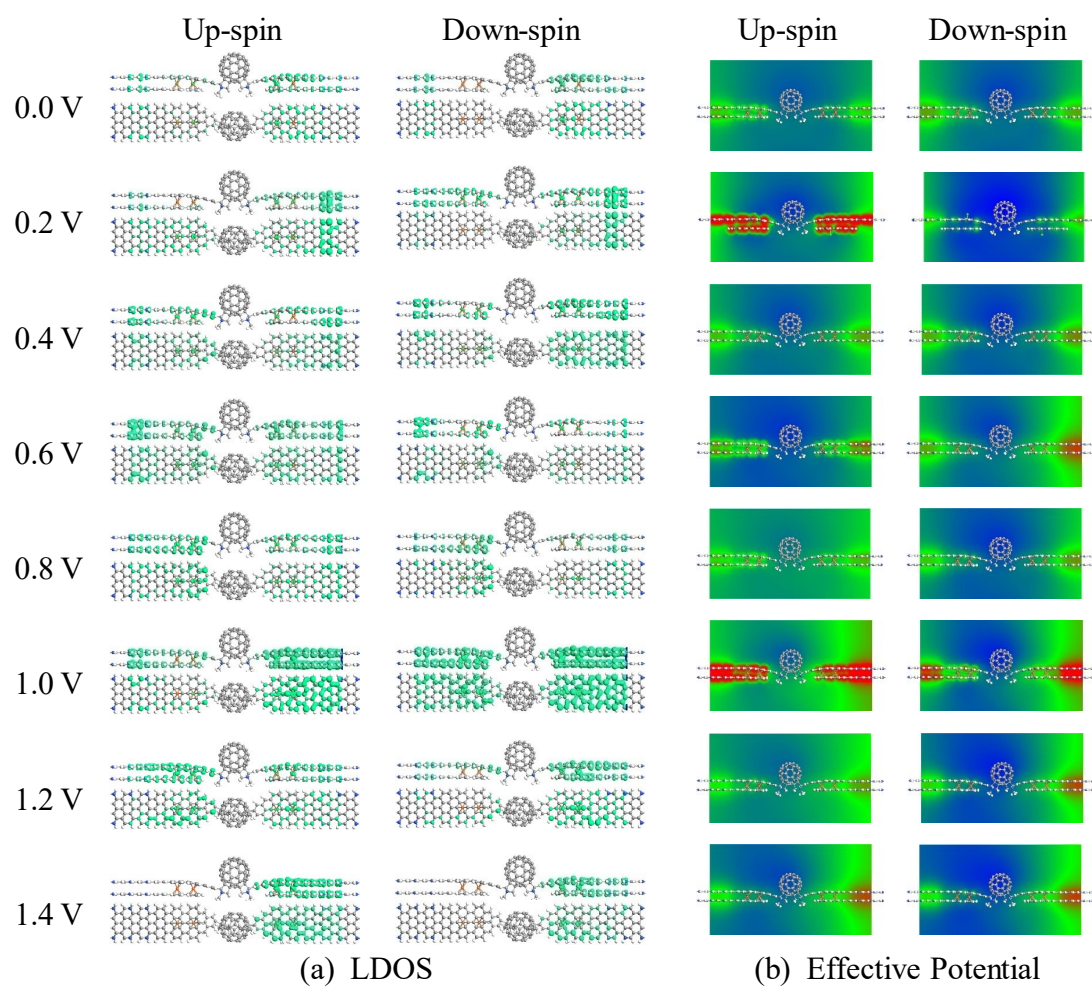


Figure S14 Spin-resolved (a) LDOS and (b) effective potentials of the **ABIIA'B'** device under various biases.