Supplied materials

Modulating multi-functional molecular devices in Zigzag Gallium Nitride Nanoribbons by different magnetic orderings : First-principles study

Tong Chen^a*, Chengkun Guo^a, Liang Xu^a*, Quan Li^a, Kaiwu Luo^b, Desheng Liu^a, Lingling Wang^c, Mengqiu Long^d

^a School of Energy and Mechanical Engineering, Jiangxi University of Science and Technology,

Nanchang 330013, China

^b Physical and Electronic Engineering Department, Tongren University, Tongren 554300,

Guizhou, China

° School of Physics and Microelectronic and Key Laboratory for Micro-Nano Physics and

Technology of Hunan Province, Hunan University, Changsha 410082, China

^d Hunan Key laboratory of Super Micro-structure and Ultrafast Process, Central South University,

Changsha 410083, China

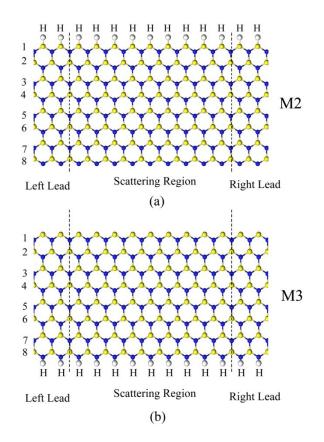


Fig. S1. (a-b) Schematic of the model devices of M2 and M3. The region outside the two dashed lines indicate the leads with two repeated carbon unit cells along the transport direction.

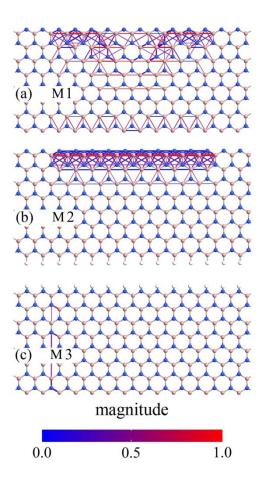


Fig. S2. (a-c)The total spin transmission pathways of M 1, M 2, and M 3 with P spin configuration at Fermi energy, respectively.

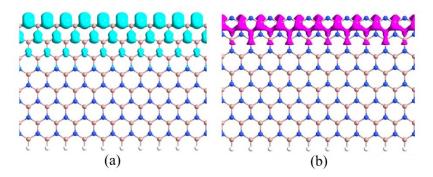


Fig. S3. The isosurfaces of spin density for M 2 with P and AP-1 spin configurations, in which the acid blue and roland purple colors present the spin down and spin up states, respectively.