

Supplementary Information for
Driving Interference control by side carbon chain in
molecular and two dimensional nano-constrictions

Dawei Kang^{1,*}, Weiwei Ju¹, Shuai Zhang¹ and Caijuan Xia²

¹*School of Physics and Engineering, Henan University of Science and Technology, Luoyang 471023, China*

²*School of Science, Xi'an Polytechnic University, Xi'an 710048, China*

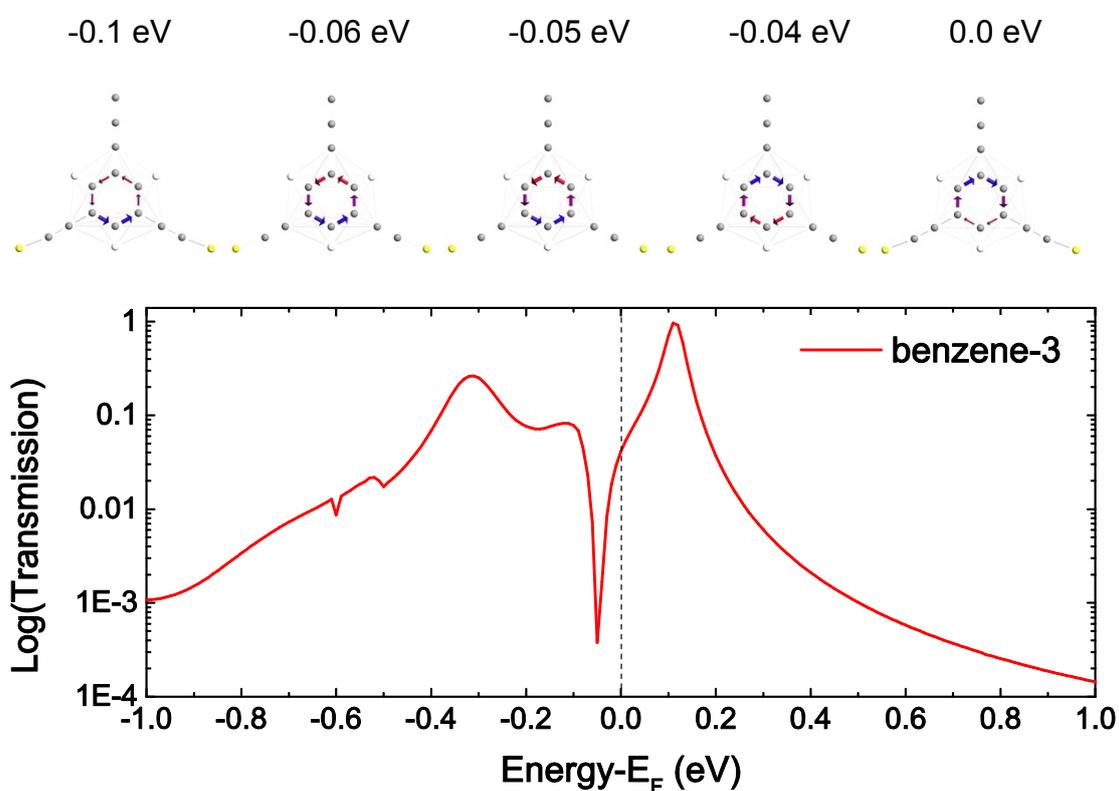


Fig.S1. The logarithm of transmission and interatomic transmission pathway analysis of the benzene molecular device connect with a 4-atom-length side carbon chain. The dip of transmission is located at -0.05 eV. The local transmission pathways at five energy points sampled symmetrically around the dip is plotted above the transmission spectrum plot.

* kdw@haust.edu.cn

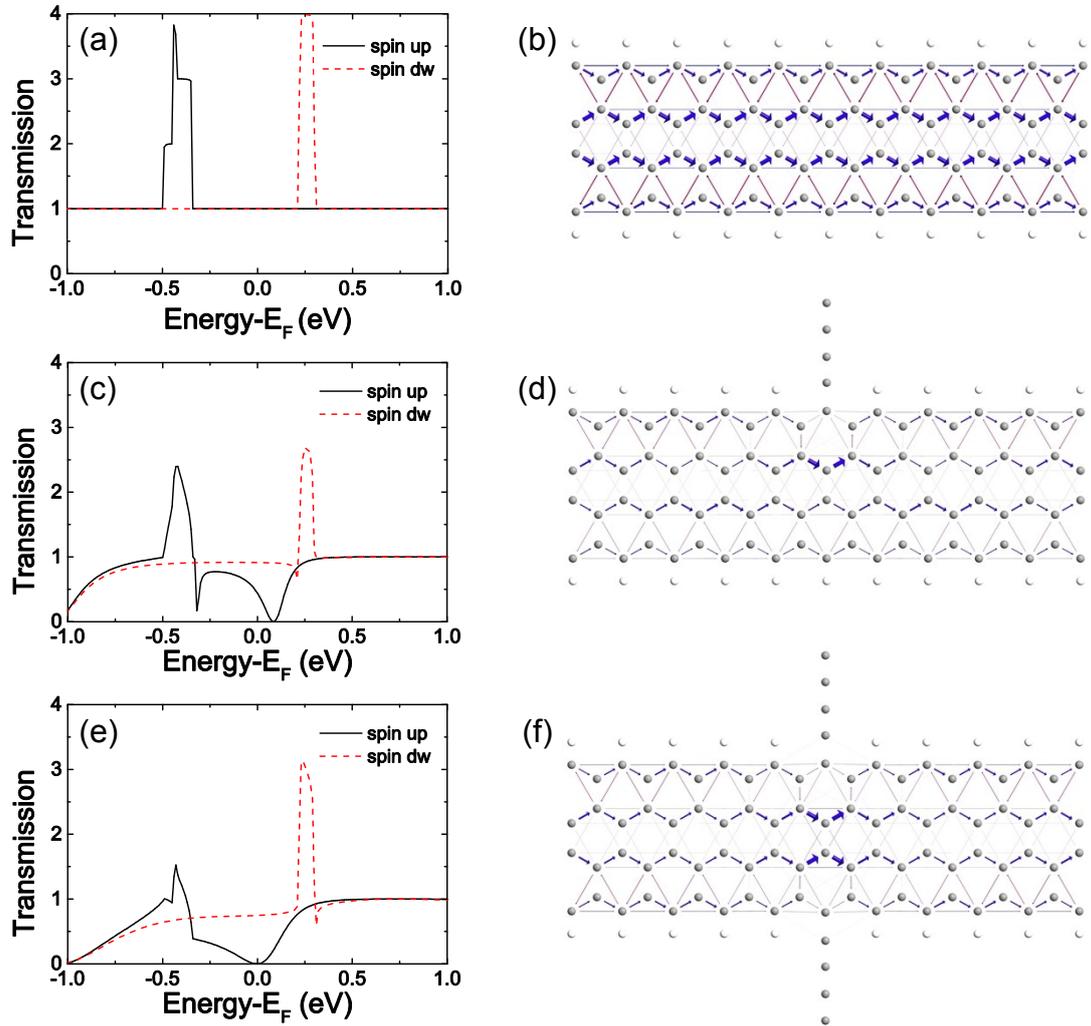


Fig.S2 The spin dependent transmission spectrum of (a) pristine 4-ZGNR, (c) the 4-ZGNR connected with one 4-atom-length side carbon chain at the upper edge and (e) the 4-ZGNR connected with two 4-atom-length carbon chain at both edges. Interatomic transmission pathway analysis for spin down state is plotted in (b), (d) and (f) corresponding to the spin down transmission in (a), (c) and (e) at Fermi energy respectively.

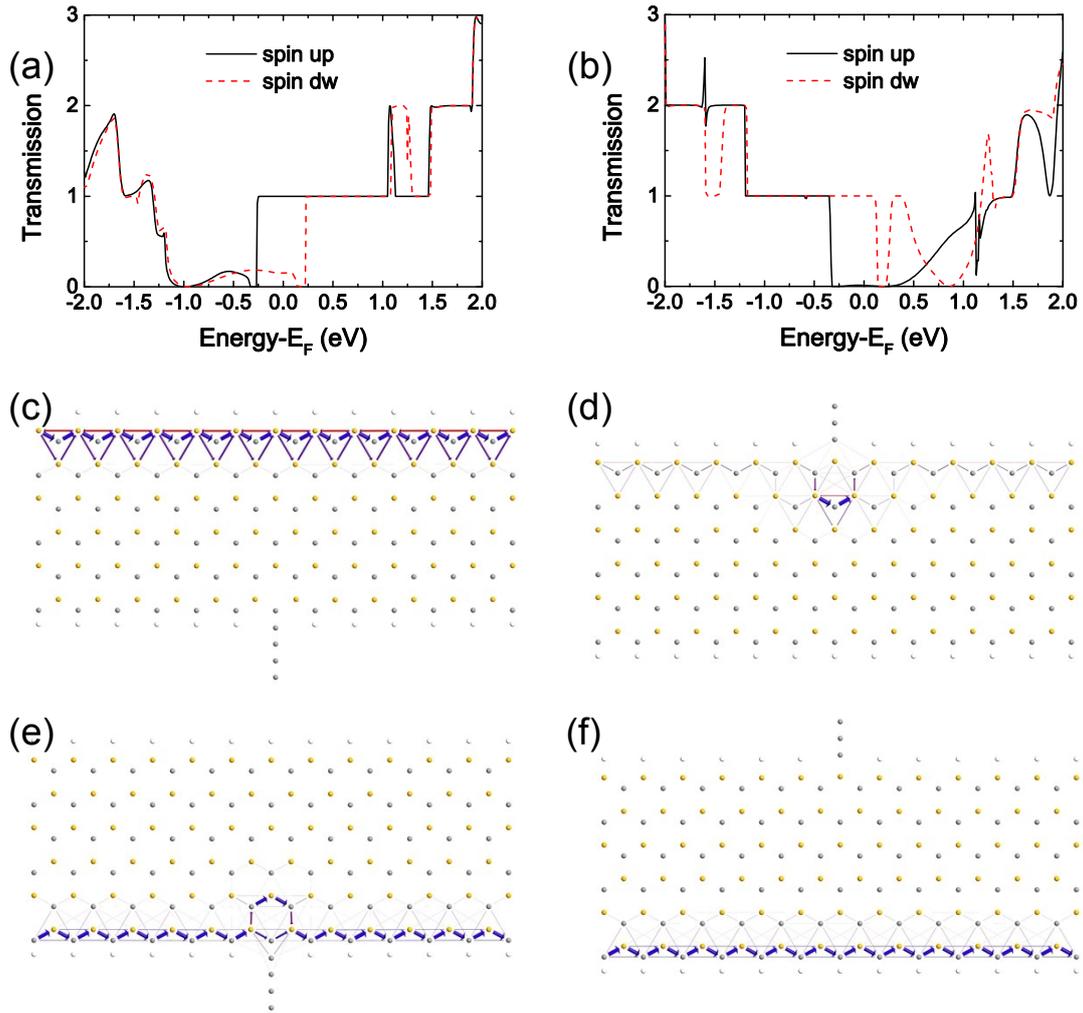


Fig.S3 The spin dependent transmission spectrum of (a) the 6-SiCNR connected with a 4-atom-length side chain at the lower all carbon edge and (b) the 6-SiCNR connected with a 3-atom-length side chain at the upper all silicon edge. Interatomic transmission pathway analysis at Fermi energy is plotted in (c, d, e, f). Note that (c) and (e) is corresponding to the spin up and down transmission at Fermi energy in (a), while (d) and (f) is corresponding to the spin up and down transmission at Fermi energy in (b).

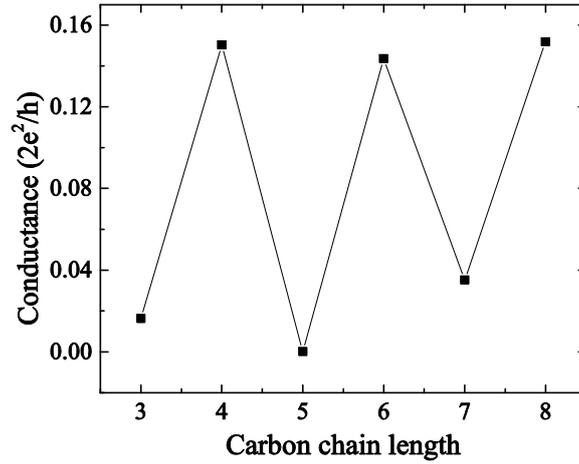


Fig.S4 The dependence of spin down transmission at Fermi energy on the length of the side carbon chain for 6-SiCNR connected by side carbon chain at the lower all carbon edge.

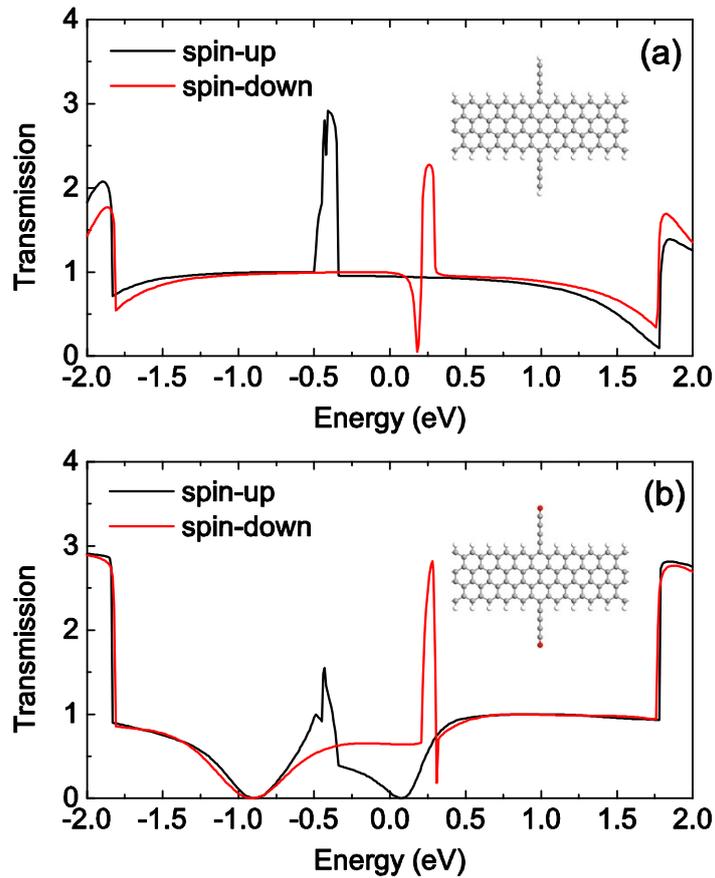


Fig.S5 The passivation effect on the transmission spectrum of ZGNR device. The 4-ZGNR connected with two 4-atom-length side carbon chains at both edges where the dangling bond of ending carbon atom in the side carbon chain is saturated by (a) a hydrogen atom and (b) an oxygen atom.

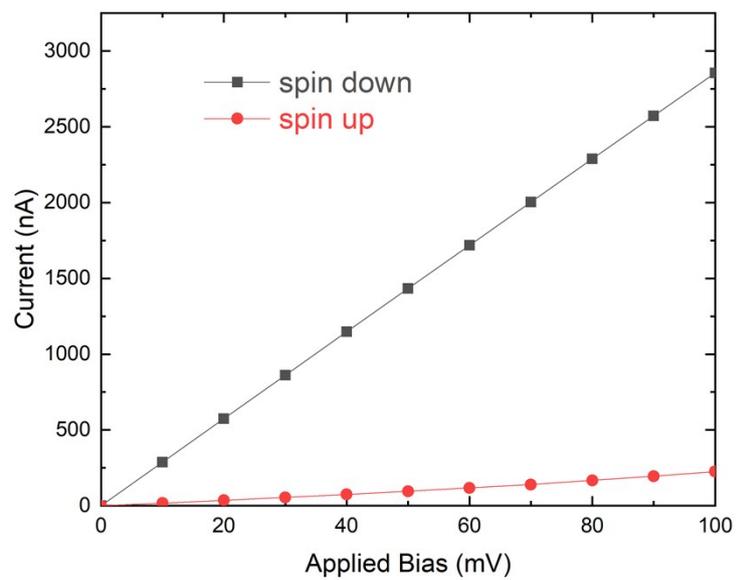


Fig.S6 The current-voltage curves of the 4-ZGNR connected with two 4-atom-length side carbon chains at both edges