Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Uniformly and perfectly linear current-voltage characteristics of nitrogen-doped armchair graphene nanoribbons for nanowires

Lingling Liu,[a] Xiao-Fei Li,[*a] Qing Yan,[a] Qin-Kun Li,[a] Xiang-Hua Zhang,[a] Mingsen Deng,[b] Qi Qiu,[a] and Yi Luo [b,c,d]

[a] School of Optoelectronic Information, University of Electronic Science and Technology of China, Chengdu, Sichuan, 610054, P. R. China

[b] Guizhou Synergetic Innovation Center of Scientific Big Data for Advanced Manufacturing Technology, Guizhou Education University, Guiyang, 550018, China

[c] Hefei National Laboratory for Physical Science at the Microscale, University of Science and Technology of China, Hefei, Anhui 230026, P. R. China.

[d] Department of Theoretical Chemistry and Biology, School of Biotechnology, KTH Royal Institute of Technology, S-10691 Stockholm, Sweden.

** e-mail: xf.li@uestc.edu.cn*

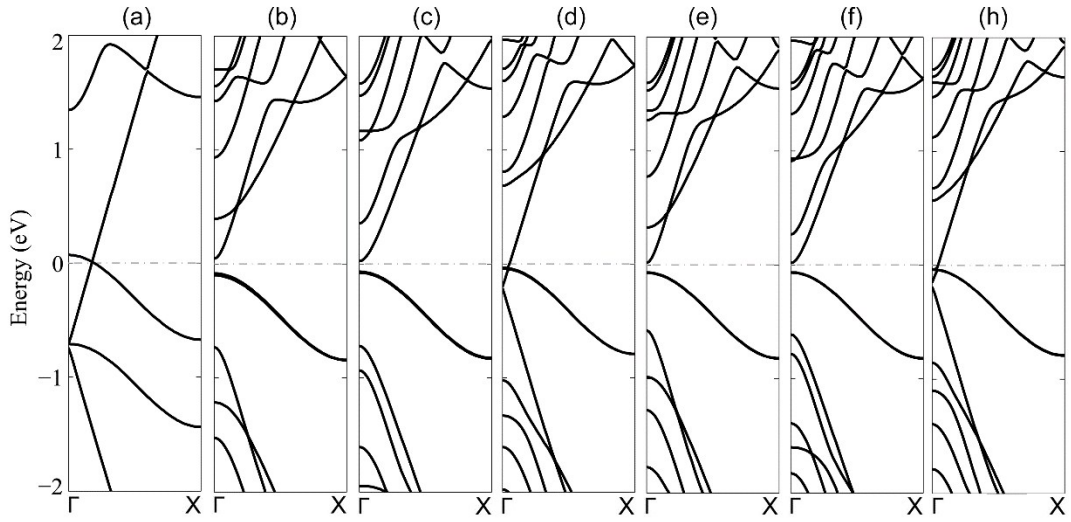

Figure S1 | the calculated band structure of the double-edge nitrogen-doped AGNRs with the width of (a) n=5, (b) n=12, (c) n=13, (d) n=14, (d) n=15, (e) n=16, and (h) n=17, respectively.

From the Figures, one can found the features: (i) All the AGNRs in the family with the width n=3p+2 are metallic, and all the AGNRs in other two families with the width n=3p or 3p+1 are semiconducting. (ii) The two delocalized impurity-bands for the narrowest one with n=5 split widely due to the strong quantum confinement effect. (iii) With the width increases, the two bands move close to each other and the band gap reduces due to the gradually reduced quantum confinement reduces.