## **Supplementary Information**

## Electronic and optical properties of surface-functionalized armchair graphene nanoribbons

Min Wang,<sup>\*ab</sup> Si Xing Song,<sup>ab</sup> Hai Xing Zhao,<sup>ab</sup> Yu Chen Wang<sup>ab</sup>

<sup>a</sup>Institute for Clean Energy & Advanced Materials, Faculty of Materials and Energy,

Southwest University, Chongqing 400715, P. R. China. Email:minwang@swu.edu.cn

<sup>b</sup>Chongqing Key Laboratory for Advanced Materials and Technologies of Clean

Energies, Chongqing 400715, P. R. China

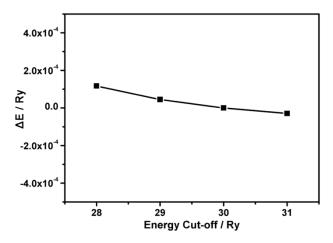


Fig. S1 The energy difference versus different energy cut-off.

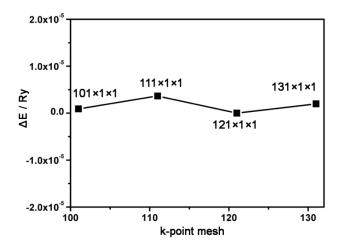


Fig. S2 The energy difference versus different k-point mesh.

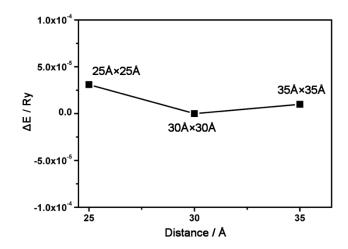


Fig. S3 The energy difference versus different separation along y and z direction.