## **Electronic Supplementary Information**

## N-substituted defective graphene sheets: promising electrode materials for Na-ion batteries

Hao Shen,<sup>a</sup> Dewei Rao,<sup>\*a</sup> Xiaoming Xi,<sup>b</sup> Yuzhen Liu,<sup>\*c</sup> and Xiangqian Shen<sup>ab</sup>

<sup>*a*</sup> Institute for Advanced Materials, School of Materials Science and Engineering, Jiangsu University, Zhenjiang 212013, P. R. China. E-mail: dewei@ujs.edu.cn.

<sup>b</sup> Changsha Research Institute of Mining and Metallurgy Co., Ltd, No. 966 South Lushan Road, Changsha, 410012, P. R. China.

<sup>c</sup> Department of Applied Physics, Nanjing University of Science and Technology, Nanjing 210094, PR China. E-mail: yzliu@njust.edu.cn.



Fig. S1 The optimized structure of pristine graphene, GG, PIG and PRG.



Fig. S2 The distance between Na and surrounding C/N atoms.



**Fig. S3** The charge distribution of Na adsorbed on pristine graphene, GG, PIG and PRG (Using the Bader population analysis in DMol<sup>3</sup> package).



Table S1 Detail information of 1~6 Na adsorbed structures.