## **Supplementary Information for:**

## "Strong selective oxidization on two-dimensional GaN: a

## first principle study"

Jiabo Chen, <sup>‡a,b</sup> Jiaduo Zhu, <sup>‡a,b\*</sup> Jing Ning,<sup>a,b</sup> Xiaoling Duan,<sup>a,b</sup>

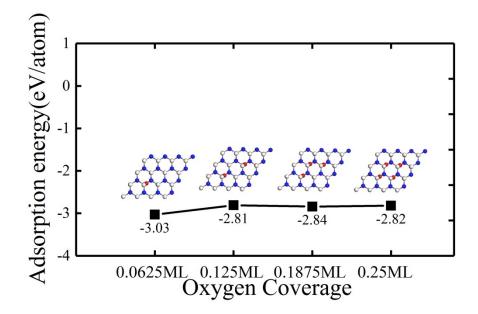
Dong Wang, <sup>a,b</sup> Jincheng Zhang<sup>a,b\*</sup> and Yue Hao<sup>a,b</sup>

Wide Bandgap Semiconductor Technology Disciplines State Key Laboratory, School of Microelectronics, Xidian University, Xi'an 710071, China

\*E-mail: jdzhu@xidian.edu.cn

## I. Oxygen Atoms Adsorbed at Gallium Surface at Low Oxygen Coverage

To signify process of oxygen atoms adsorption effect on gallium surface more generally, we adopted a  $4\times4$  supercell for implementation from 0.0625 to 0.25ML. Calculated adsorption energies and corresponding structures are shown in Fig. S1. We found that oxygen adatom still tends to take site of hydrogen atom at the top of gallium atom with adsorption energy of ~2.8eV, confirming the stability and consistency of the adsorption structures.



**Fig. S1** Adsorption energy per oxygen adatom and corresponding structures at gallium surface with low oxygen coverage.