Supplementary Materials

1.110 eV

(a)

0.450 eV

(b)

0.378 eV

(c)

-0.597 eV

(d)
Figure S1. Possible adsorption configurations for O$_2$ adsorption on the defective WO$_3$(001) surface. The bond lengths (Å) close to the adsorption site are given, and the data in the parenthesis are in relative to the defective WO$_3$(001) surface before O$_2$ adsorption. In addition, the corresponding adsorption energies have also been provided.