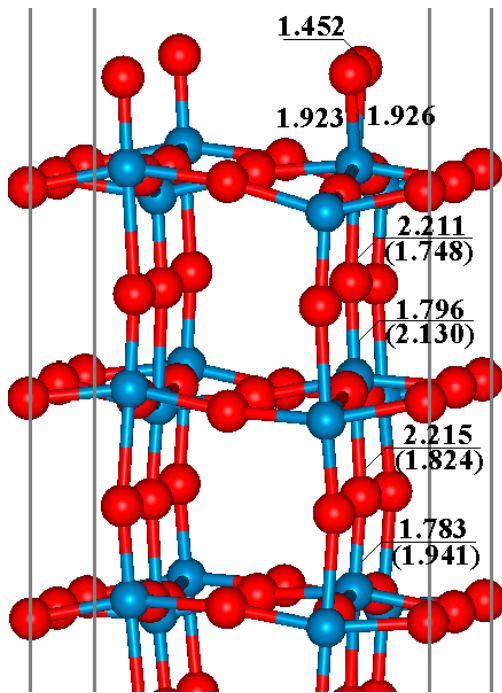
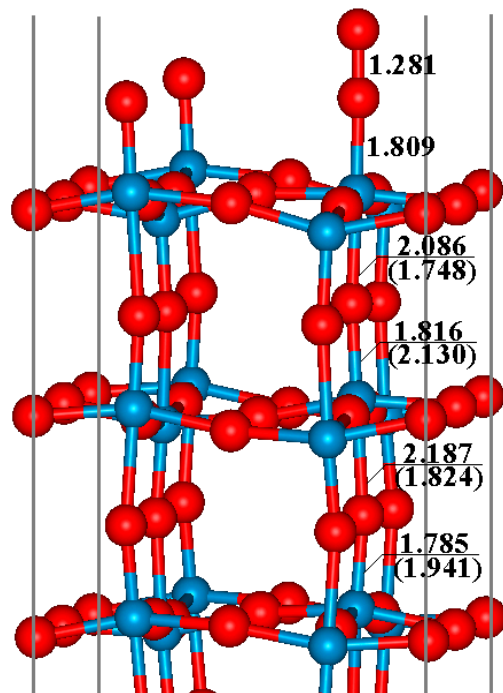


Supplementary Materials



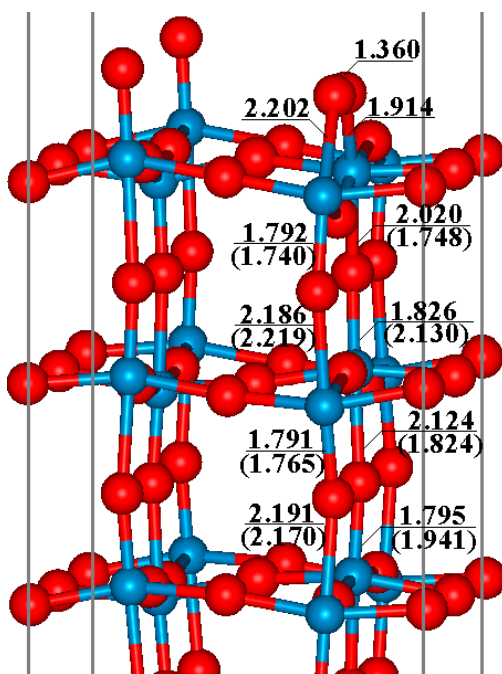
1.110eV

(a)



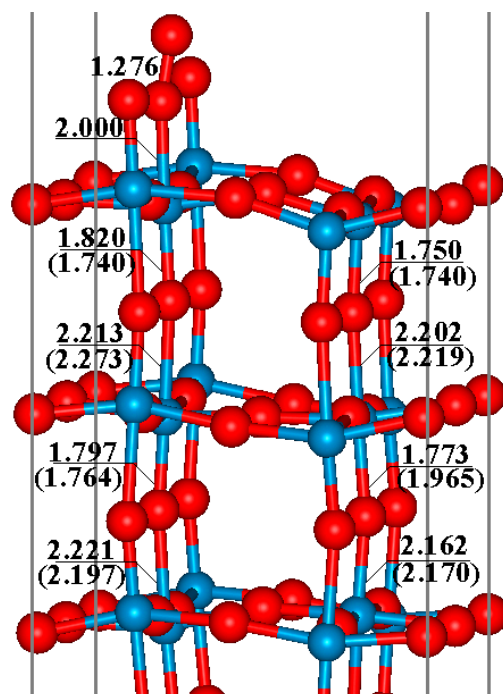
0.450eV

(b)



0.378eV

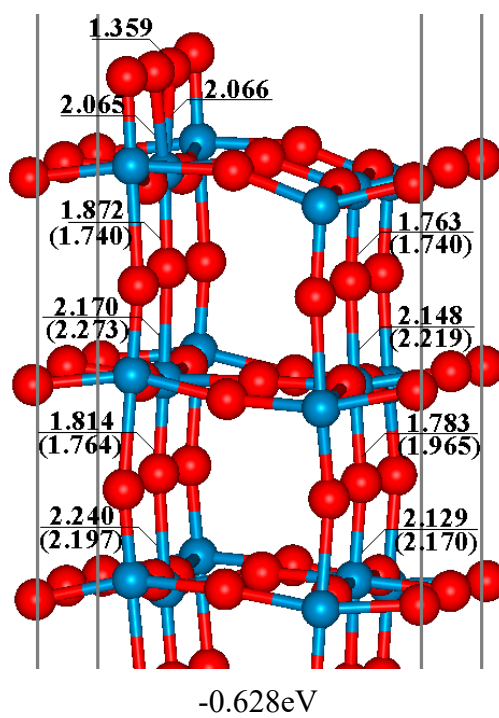
(c)



-0.597eV

(d)

Figure S1. Cont.



(e)

Figure S1. Possible adsorption configurations for O₂ adsorption on the defective WO₃(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 WO₃(001) surface before O₂ adsorption. In addition, the corresponding adsorption energies have also been provided.