

## Supporting Information

### **Fe- and Co-P<sub>4</sub>-embedded graphenes as electrocatalysts for the oxygen reduction reaction: theoretical insights**

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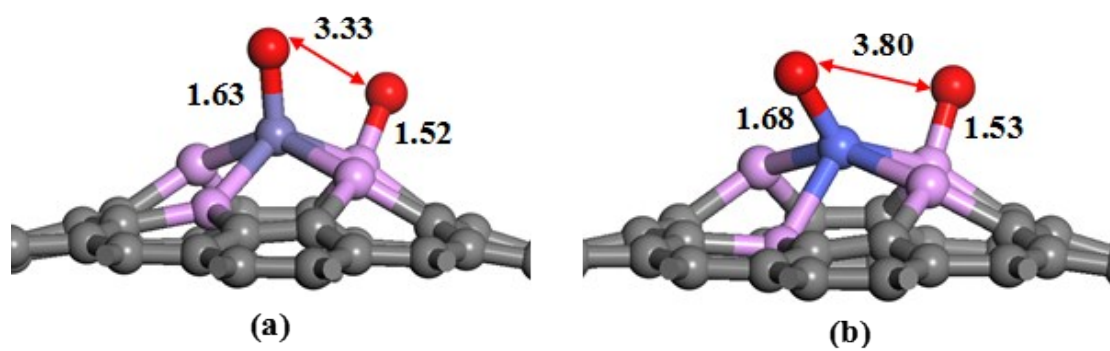
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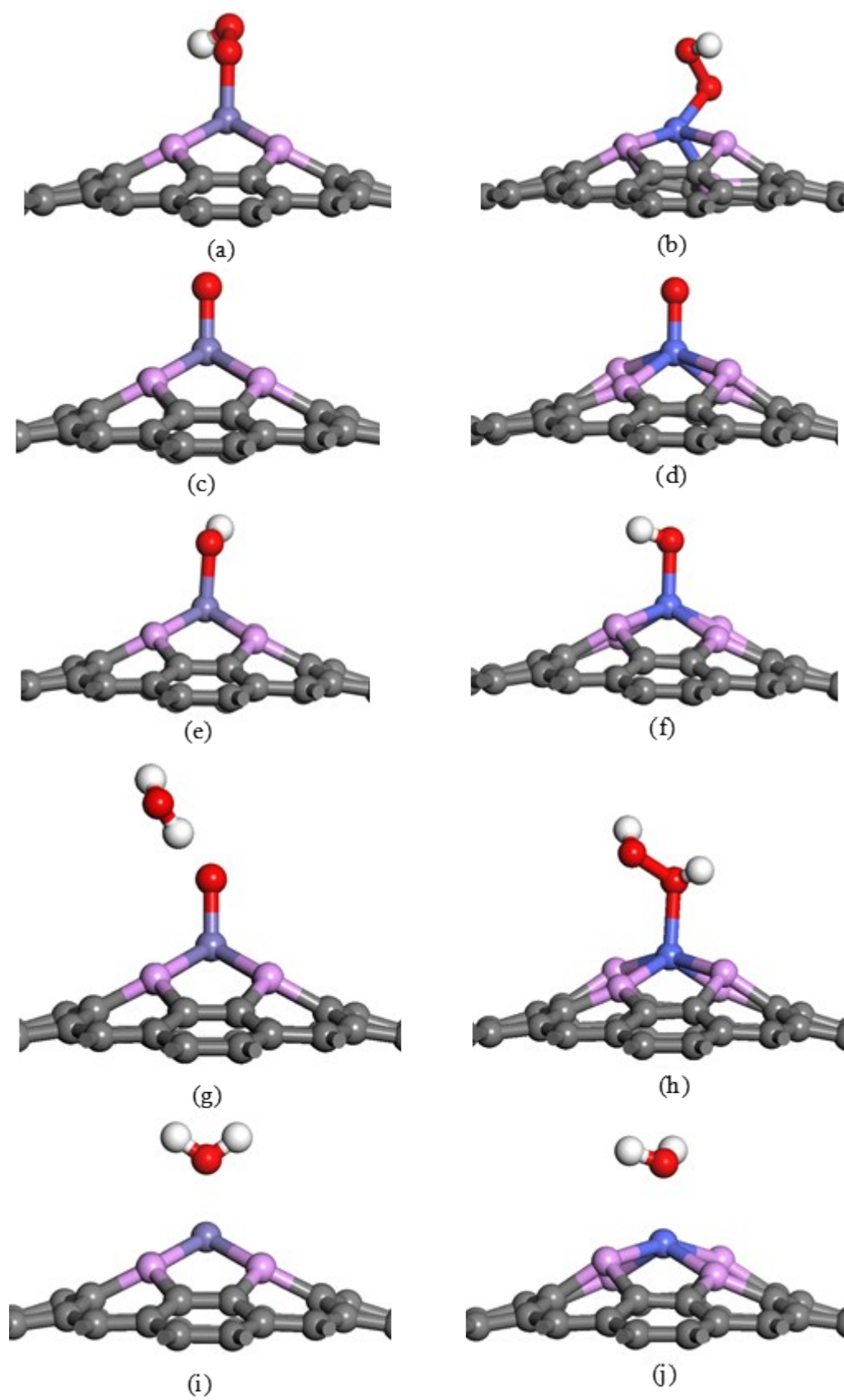
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**Table S1.** Computed adsorption energies ( $E_{\text{ads}}$ , eV) of various ORR species on the surface of Fe-P<sub>4</sub> embedded graphene in 5 × 5 and 6 × 6 supercells.

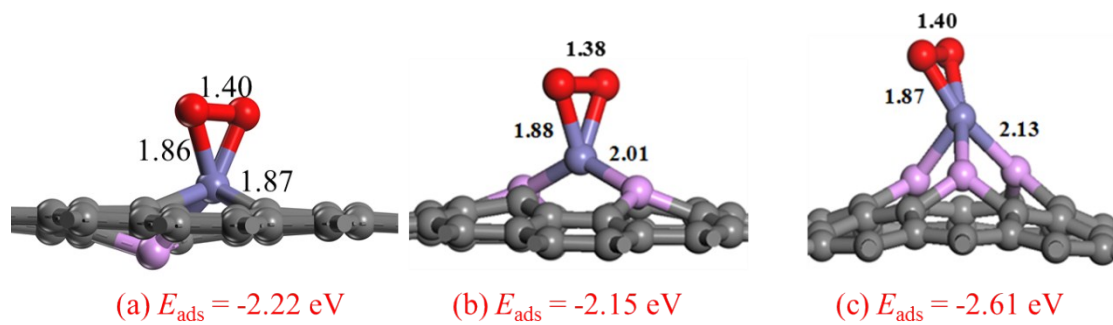
supercell	5 × 5	6 × 6
O <sub>2</sub>	-1.03	-1.03
OOH	-2.04	-2.07
OH	-3.19	-3.22
O	-4.40	-4.44
H <sub>2</sub> O	-0.42	-0.46
H	-2.61	-2.63
HOOH	-2.53	-2.55



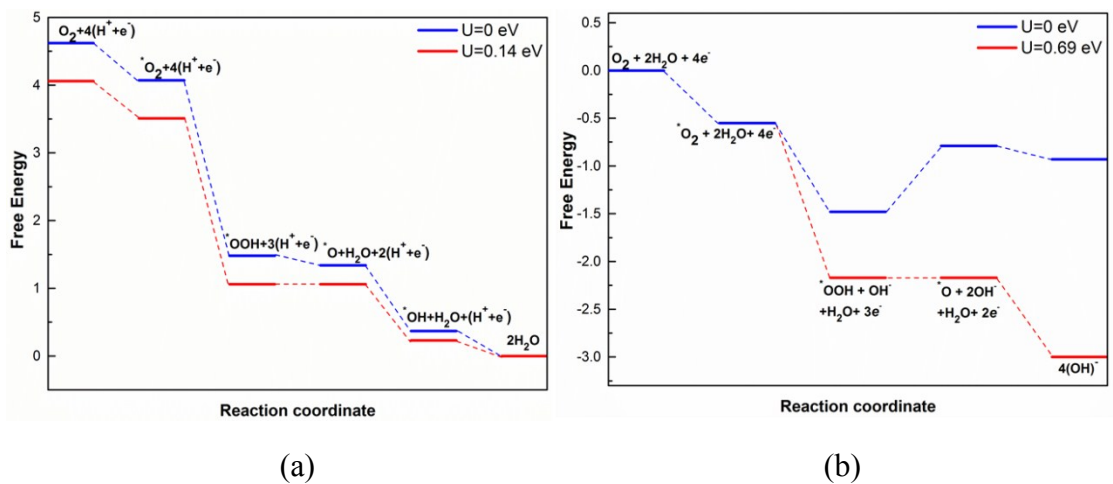
**Figure S1.** The optimized structures of the products O<sub>2</sub> dissociation on (a) Fe- and (b) Co-P<sub>4</sub> embedded graphenes.



**Figure S2.** The optimized structures of OOH, O, OH, HOOH, and H<sub>2</sub>O adsorption on Fe- (left) and Co-P<sub>4</sub> (right) embedded graphenes.



**Figure S3.** The optimized configurations of  $\text{O}_2$  adsorption on (a) Fe-P<sub>1</sub>, (b) Fe-P<sub>2</sub>, and (c) Fe-P<sub>3</sub> embedded graphenes.



**Figure S4:** Free energy diagram for the ORR on Fe- $P_4$  embedded graphene in (a) acid media and (b) alkaline media under 5% strain.