

## Supporting Information

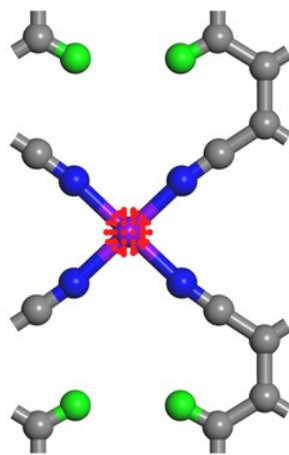
### **Two-dimensional Iron-tetracyanoquinodimethane (Fe-TCNQ) Monolayer: an Efficient Electrocatalyst for the Oxygen Reduction Reaction**

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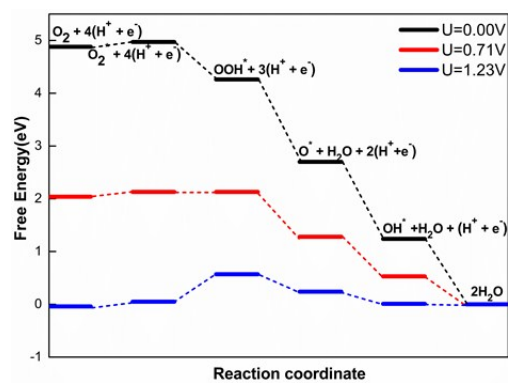
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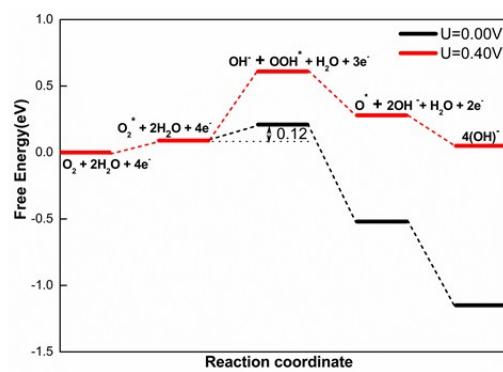
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**Fig. S1** Spin-polarized density for Fe-TCNQ monolayer with isovalue of 0.01 electrons  $\text{\AA}^{-3}$ .



(a)



(b)

**Fig. S2** Free energy diagrams for the ORR on Br-Fe-TCNQ monolayer in (a) acidic and (b) alkaline media.