Supporting Information

The oxygen reduction reaction mechanism on Sn doped graphene as an electrocatalyst in fuel cells: A DFT study

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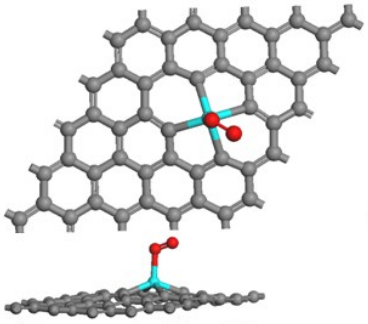
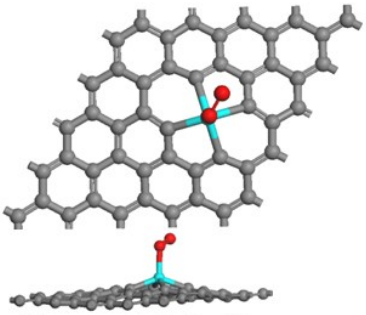
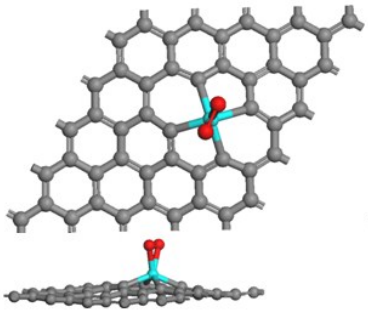
Optimized adsorption structure --- O_2



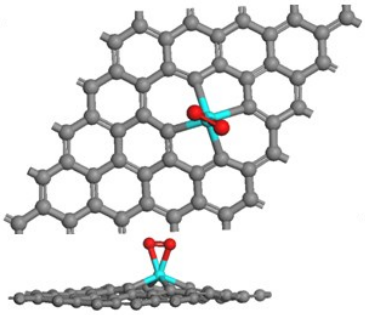
E_{ads}= -0.40 eV



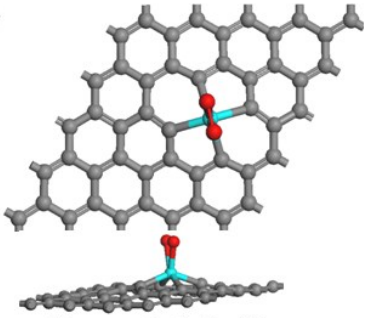
E_{ads}= -0.36 eV



E_{ads}= 0.15 eV

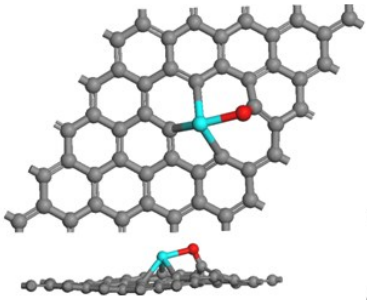


E_{ads}= 0.15 eV

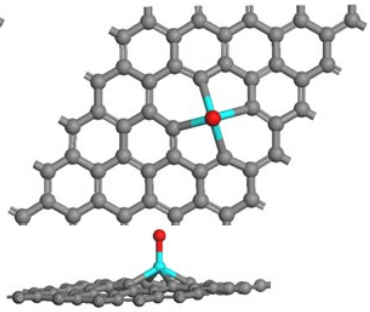


E_{ads}= 0.16 eV

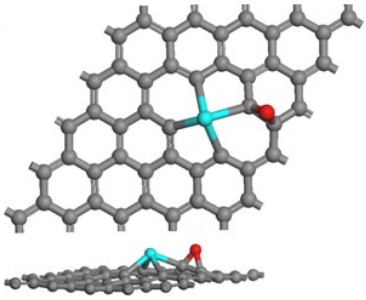
Optimized adsorption structure --- O



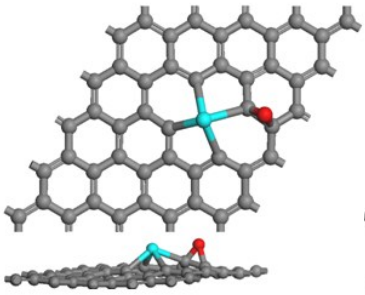
E_{ads}= -4.64 eV



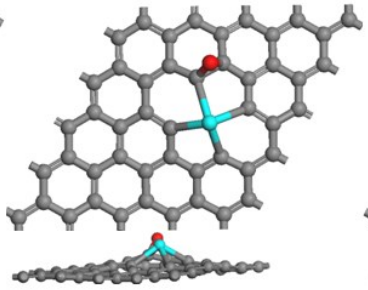
E_{ads}= -3.29 eV



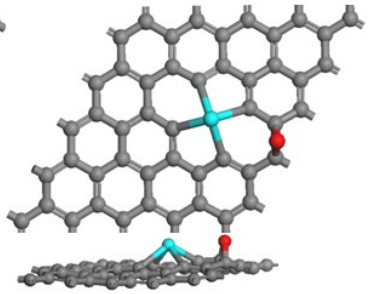
E_{ads}= -2.92 eV



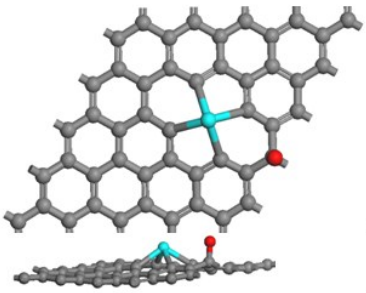
E_{ads}= -2.92 eV



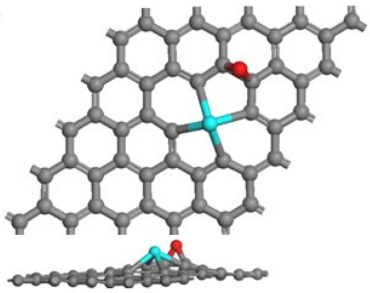
E_{ads}= -2.88 eV



E_{ads}= -2.71 eV

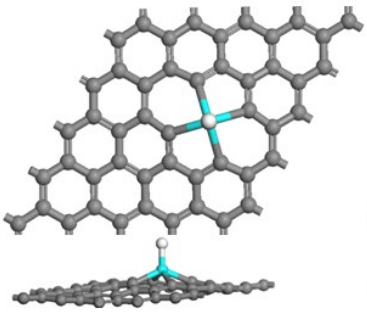


E_{ads}= -2.41 eV

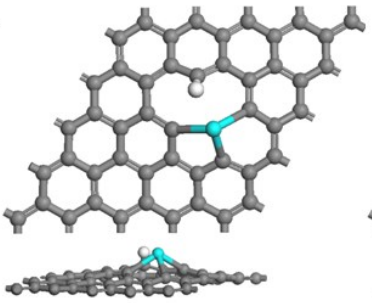


E_{ads}= -1.96 eV

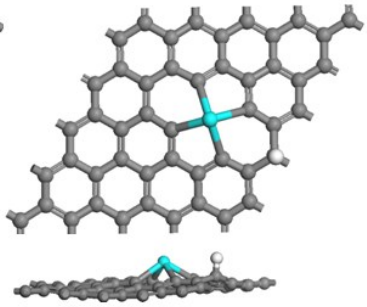
Optimized adsorption structure --- H



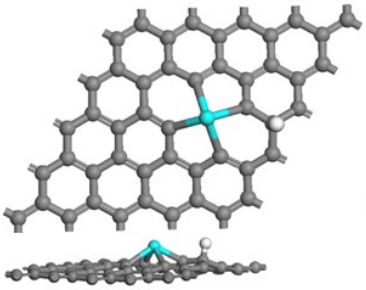
E_{ads}= -2.43 eV



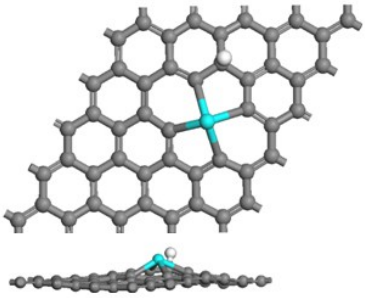
E_{ads}= -2.30 eV



E_{ads}= -1.58 eV

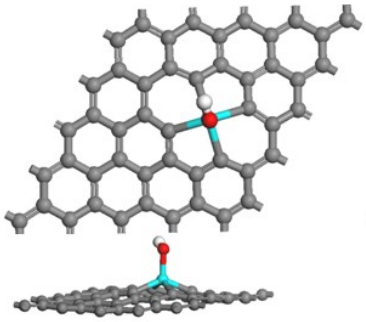


E_{ads}= -1.25 eV

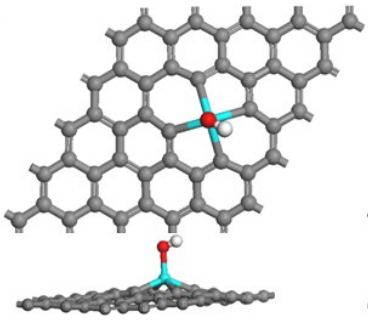


E_{ads}= -1.04 eV

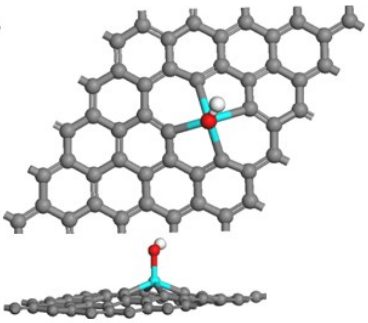
Optimized adsorption structure --- OH



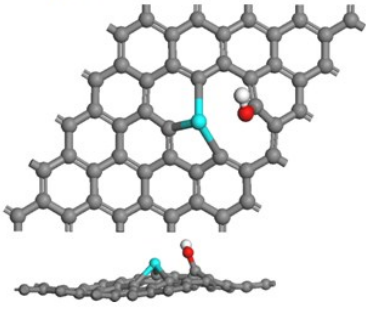
E_{ads}= -3.29 eV



E_{ads}= -3.29 eV

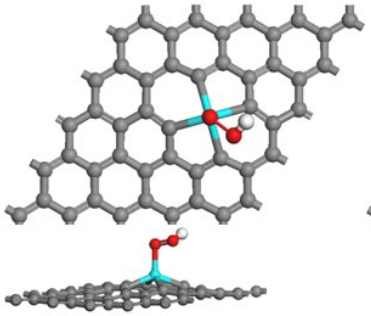


E_{ads}= -3.28 eV

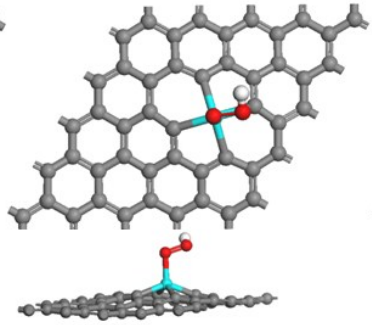


E_{ads}= -2.14eV

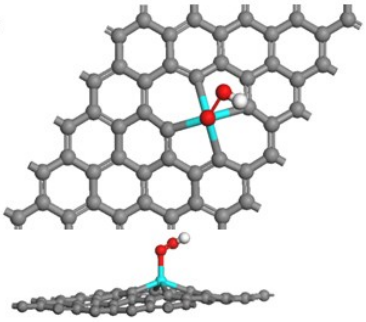
Optimized adsorption structure --- OOH



E_{ads}= - 1.69 eV

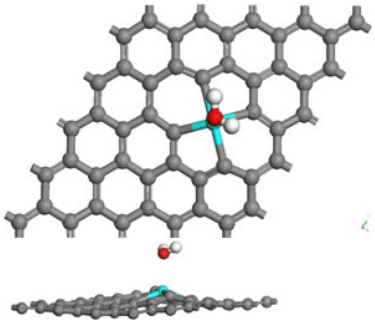


E_{ads}= - 1.67 eV



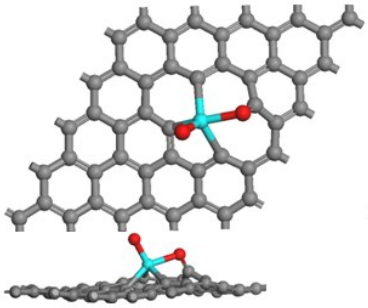
E_{ads}= - 1.65 eV

Optimized adsorption structure --- H_2O

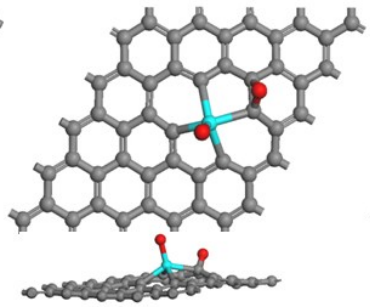


E_{ads}= -0.28 eV

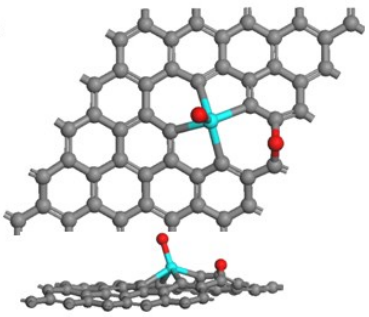
Optimized adsorption structure --- O-O



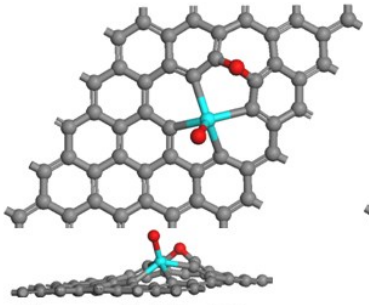
E_{ads}= -5.08 eV



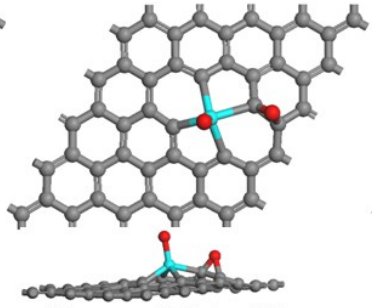
E_{ads}= - 3.35eV



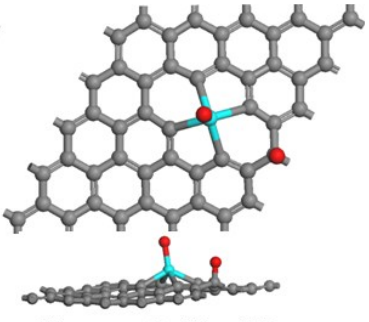
E_{ads}= - 3.32eV



E_{ads}= -3.22 eV



E_{ads}= -3.20 eV



E_{ads}= -2.51 eV

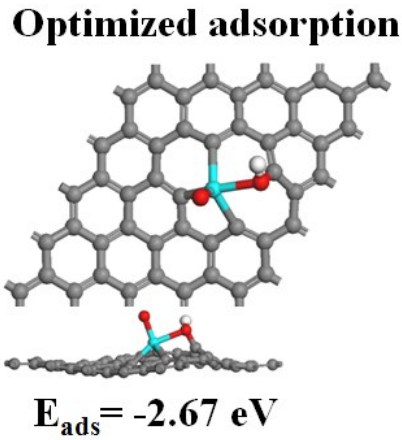


Fig. S1. Possible configurations for each adsorbed species (end-on O_2, side-on O_2, O, H, OH, OOH, H_2O, O-O and O-OH) involved in the ORR on Sn doped divacancy graphene. E_{ads} represents the adsorption energy (eV). The gray and blue balls represent C and Sn atoms, respectively.

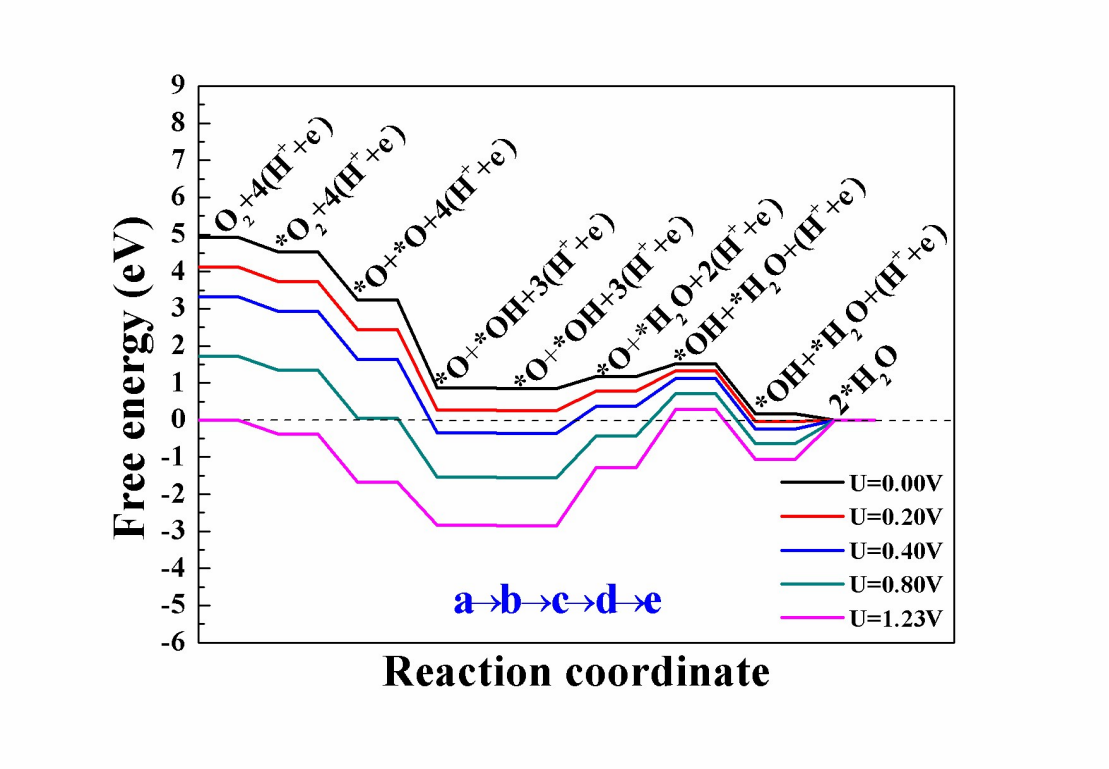


Fig. S2. The free energy diagram for the reaction pathway Ⅰ (a→b→c→d→e) on Sn doped divacancy graphene at different electrode potentials.

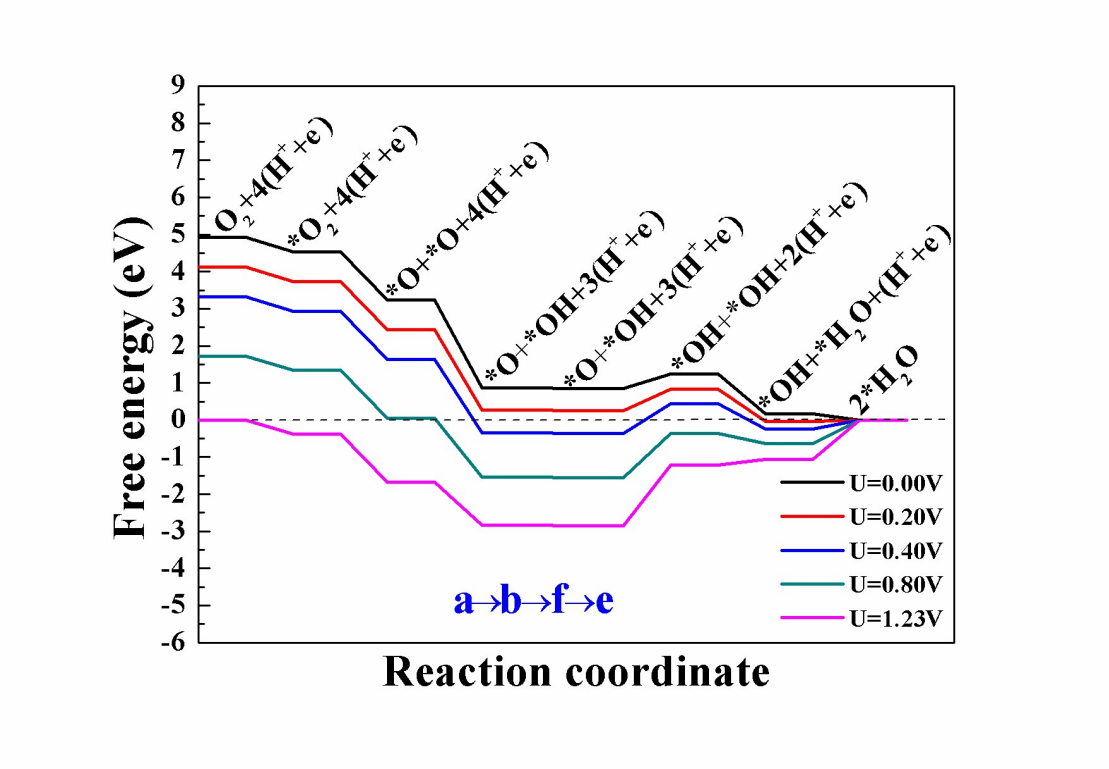


Fig. S3. The free energy diagram for the reaction pathway II (a→b→f→e) on Sn doped divacancy graphene at different electrode potentials.