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Supporting Information

Density Functional Study on the Oxygen Reduction Reaction Mechanism on FeN_2-doped Graphene

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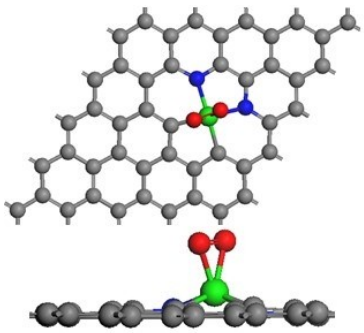
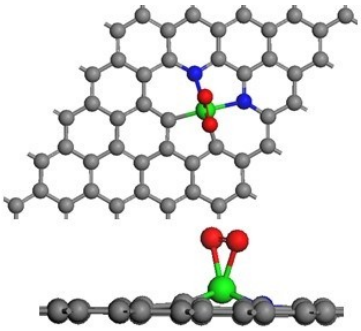
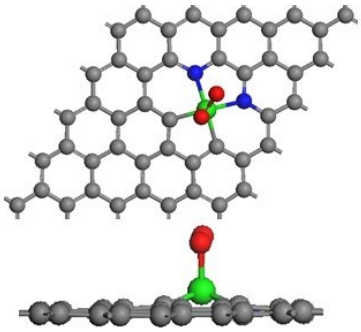
Optimized adsorption structure --- side-on O_2



ΔE_{ads}= -1.67 eV

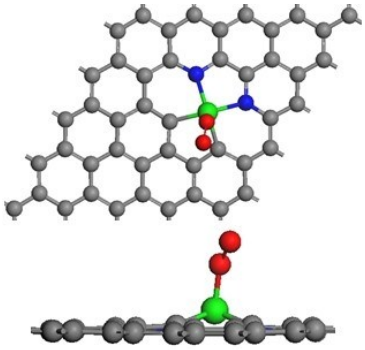


ΔE_{ads}= -1.67 eV

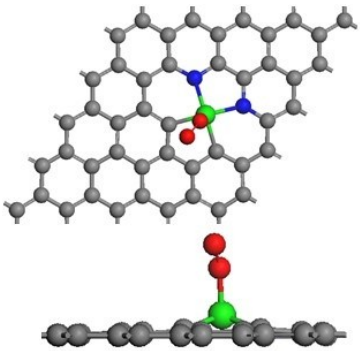


ΔE_{ads}= -1.28 eV

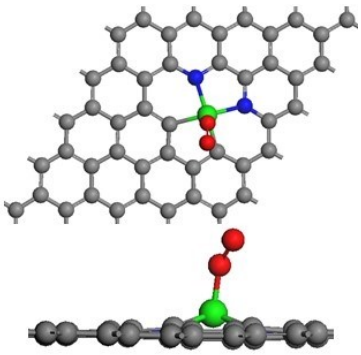
Optimized adsorption structure --- end-on O_2



ΔE_{ads}= -1.43 eV

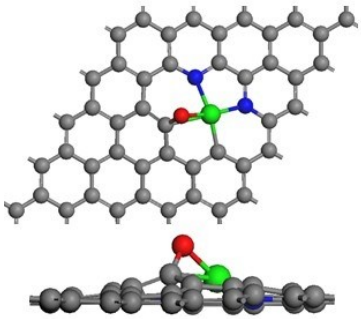


ΔE_{ads}= -1.43 eV

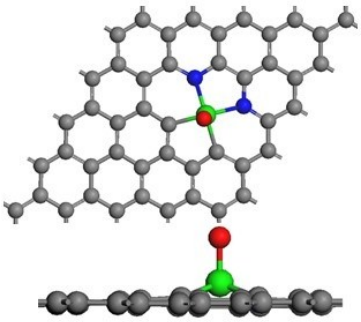


ΔE_{ads}= -1.42 eV

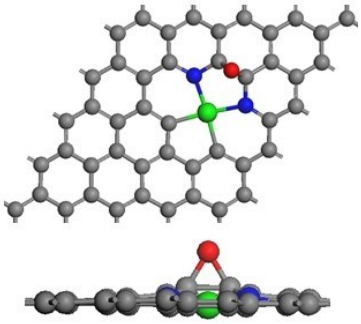
Optimized adsorption structure --- O



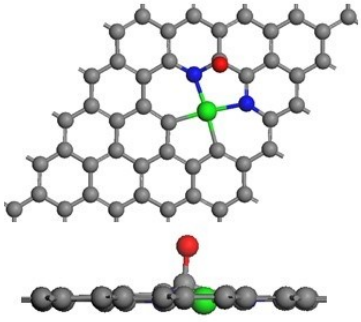
ΔE_{ads}= -5.24 eV



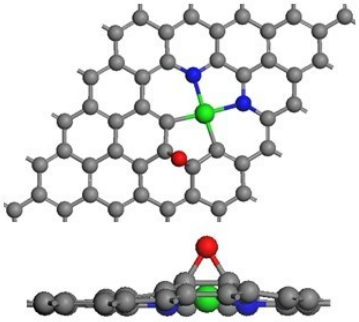
ΔE_{ads}= -4.96 eV



ΔE_{ads}= -3.03 eV

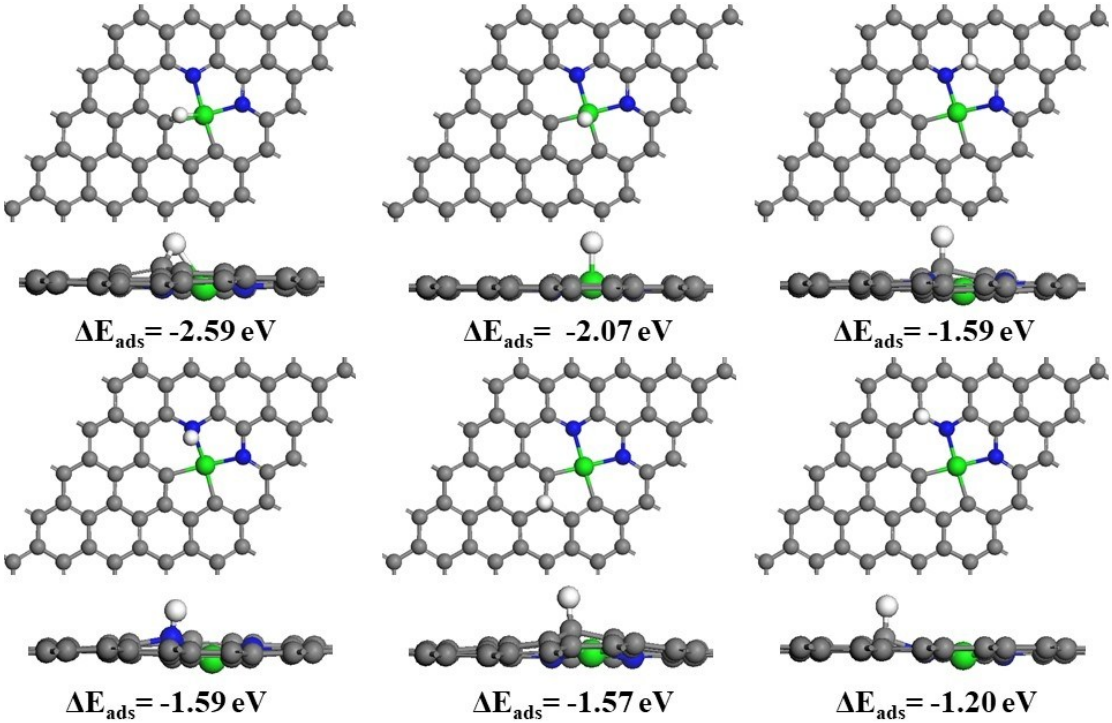


ΔE_{ads}= -2.87 eV

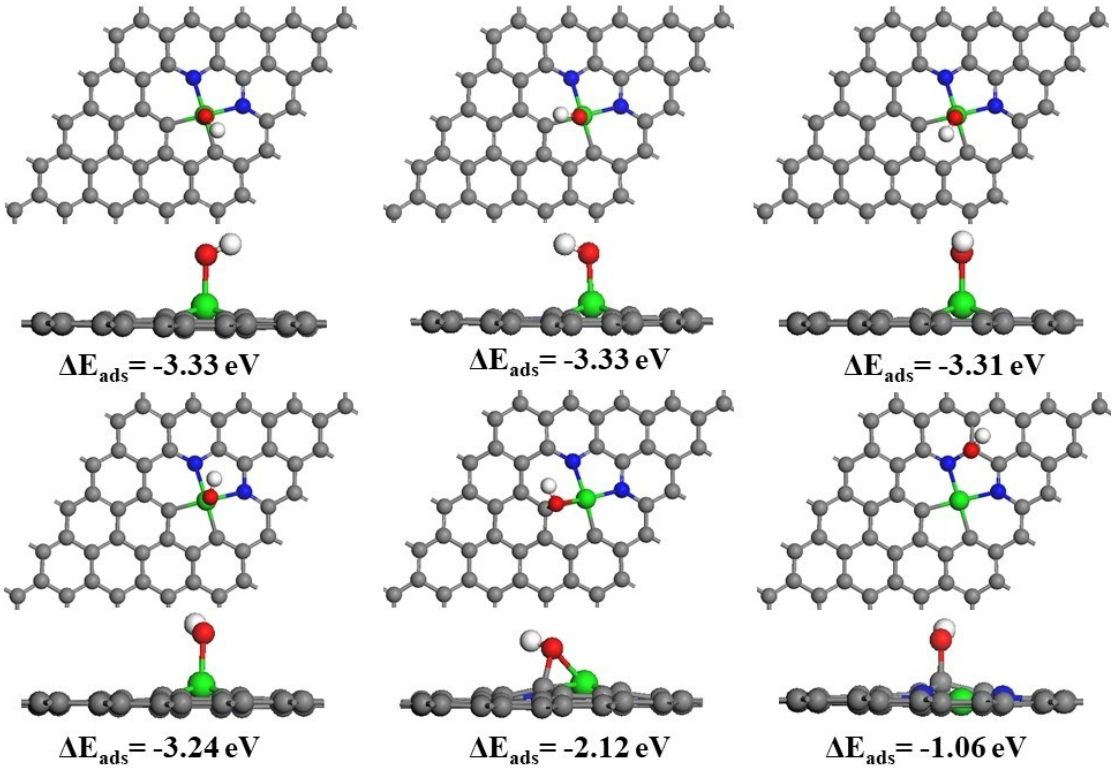


ΔE_{ads}= -2.56 eV

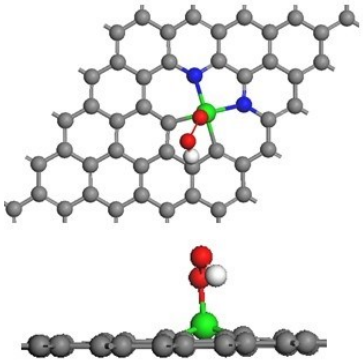
Optimized adsorption structure --- H



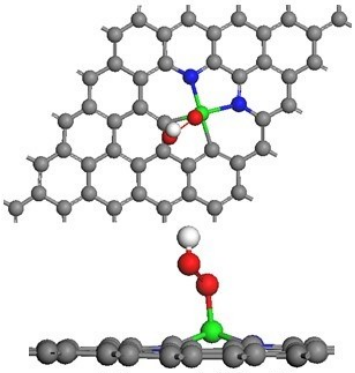
Optimized adsorption structure --- OH



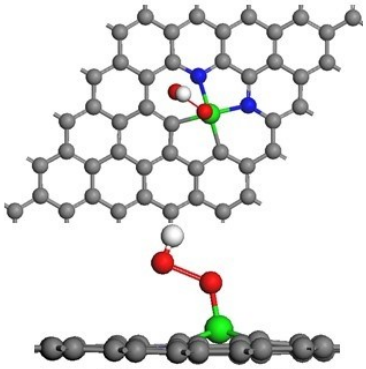
Optimized adsorption structure --- OOH



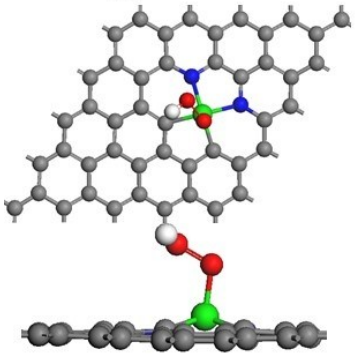
ΔE_{ads}= -1.99 eV



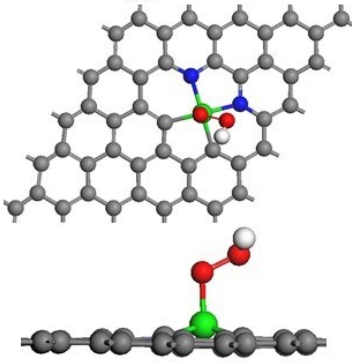
ΔE_{ads}= -1.99 eV



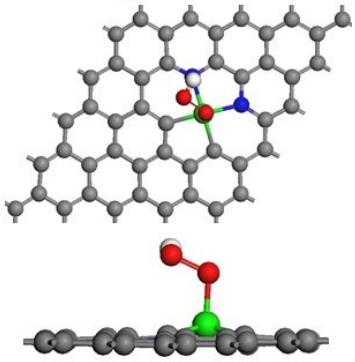
ΔE_{ads}= -1.98 eV



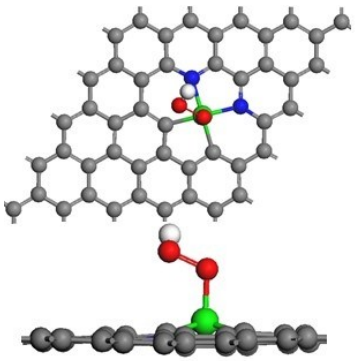
ΔE_{ads}= -1.95 eV



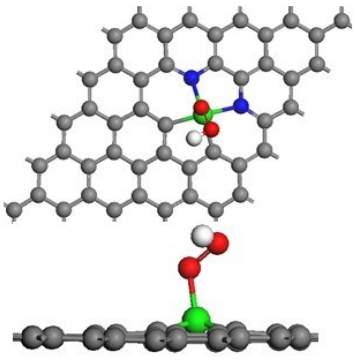
ΔE_{ads}= -1.94 eV



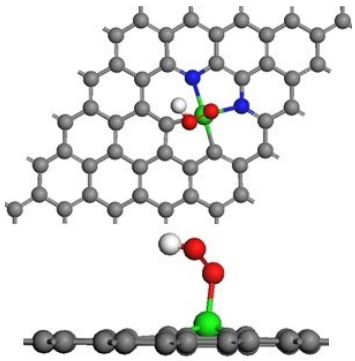
ΔE_{ads}= -1.89 eV



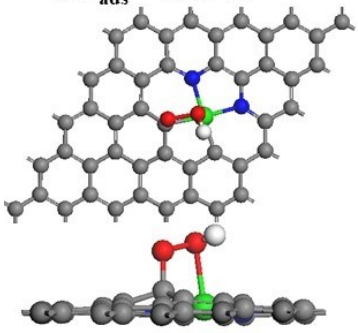
ΔE_{ads}= -1.89 eV



ΔE_{ads}= -1.87 eV

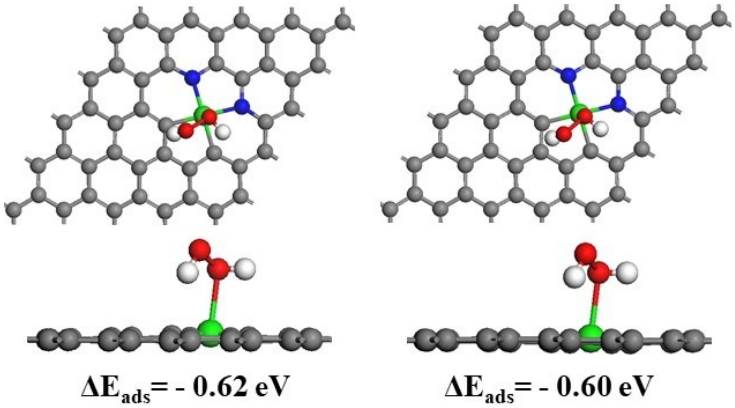


ΔE_{ads}= -1.84 eV



ΔE_{ads}= -0.99 eV

Optimized adsorption structure --- HOOH



Optimized adsorption structure --- H_2O

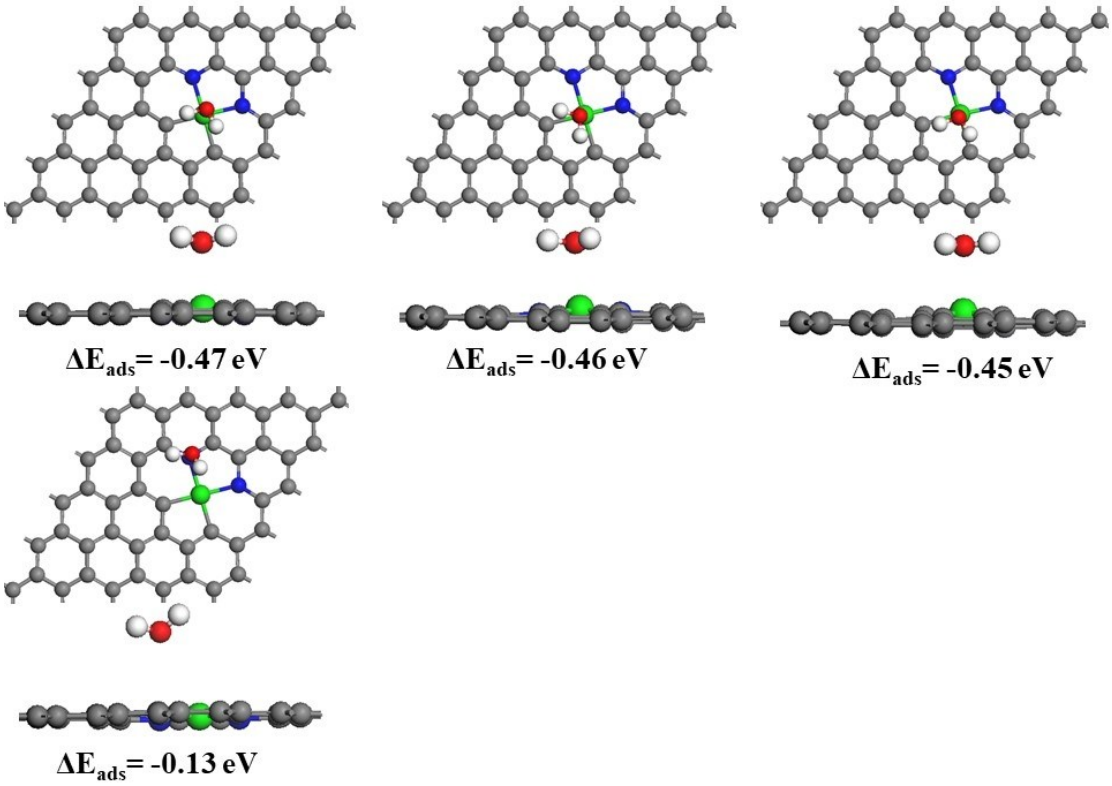
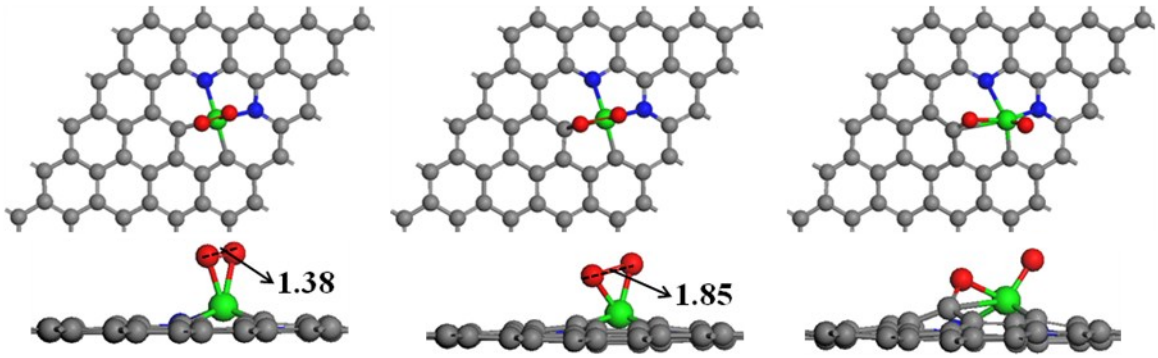
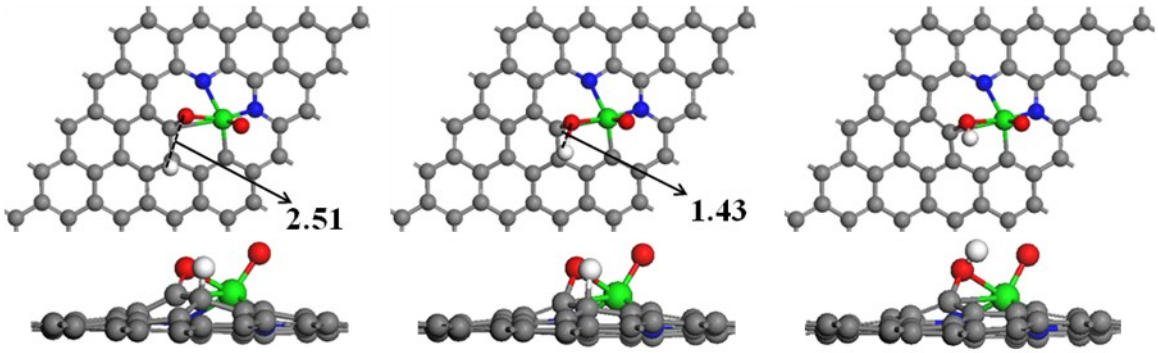


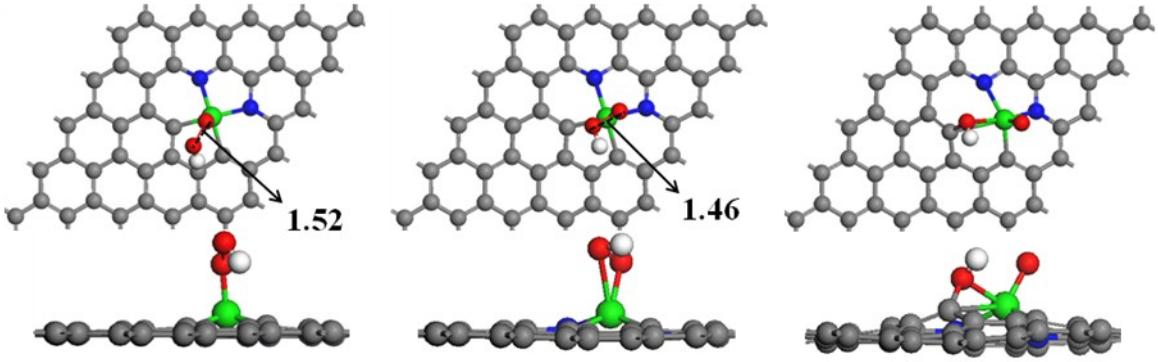
Figure S1. Possible configurations for each adsorbed species (side-on O_2, end-on O_2, O, H, OH, OOH, HOOH and H_2O) involved in the ORR. ΔE_{ads} is the adsorption energy [eV]. In the figure, the gray, blue, green, red and white balls represent C, N, Fe, O and H atoms, respectively.



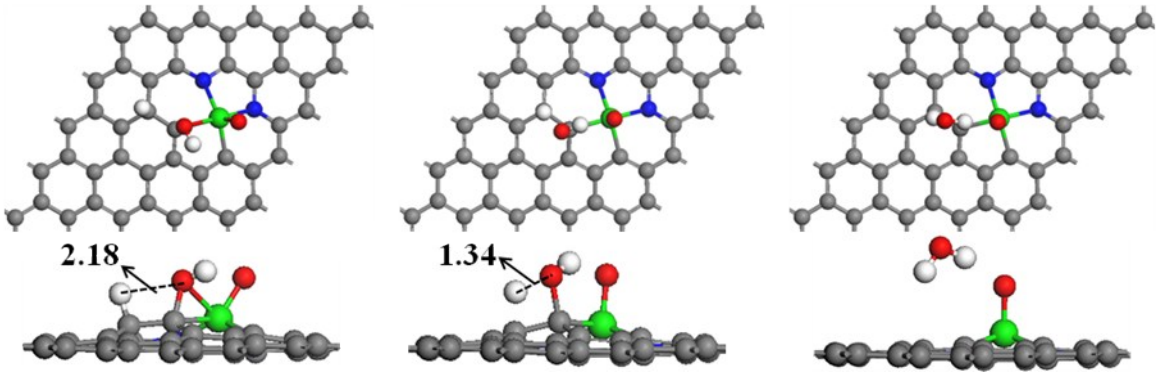
(a_1) *O_2 → *O + *O **ΔE = 1.16, ΔH= -1.14**



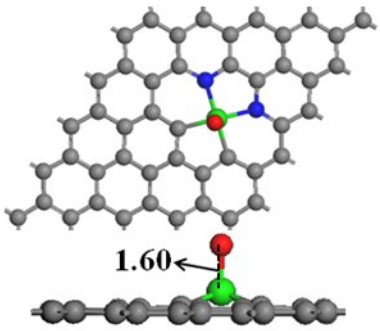
(b_1) *O + *O + *H → *OH + *O **ΔE = 1.50, ΔH= -0.40**

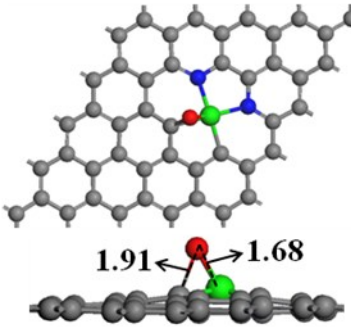


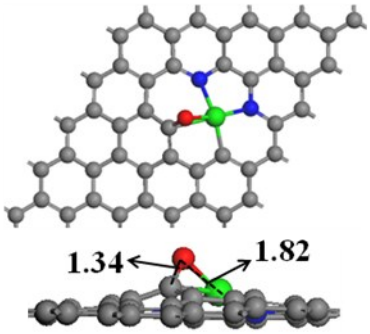
(b_2) *OOH → *OH + *O **ΔE = 0.27, ΔH = -0.96**



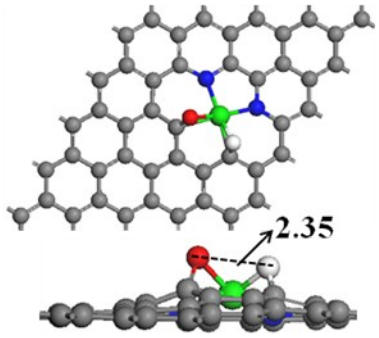
(c_1) *OH + *O + *H →*O + H_2O **ΔE = 0.29, ΔH = -2.28**

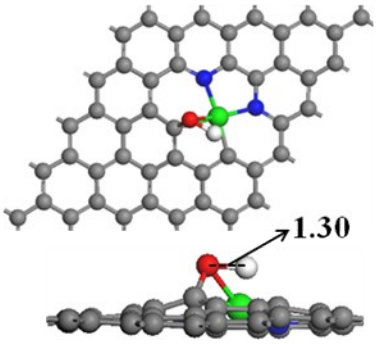


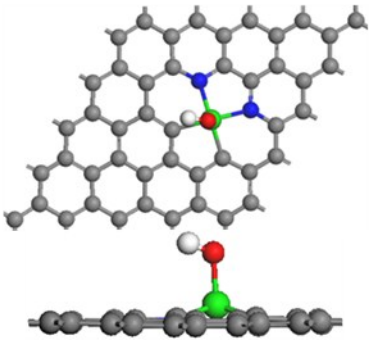




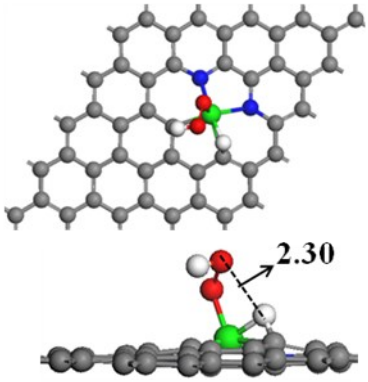
(d_1) *O (T_1) → *O (B_1) **ΔE = 0.57, ΔH = -0.29**

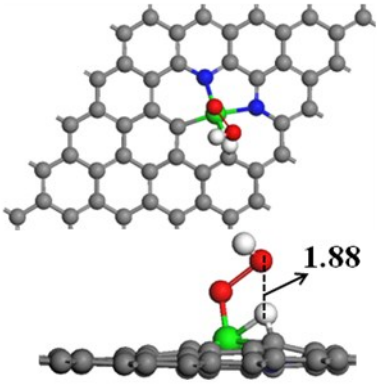


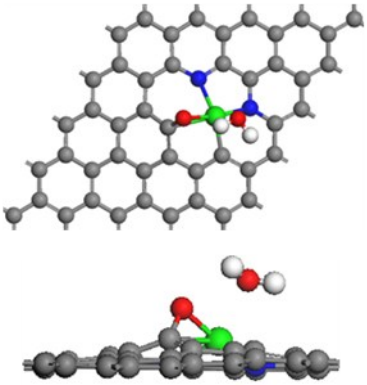




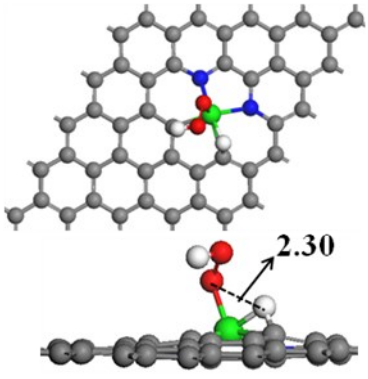
(e_1) *O + *H→ *OH **ΔE = 1.08, ΔH = -0.59**

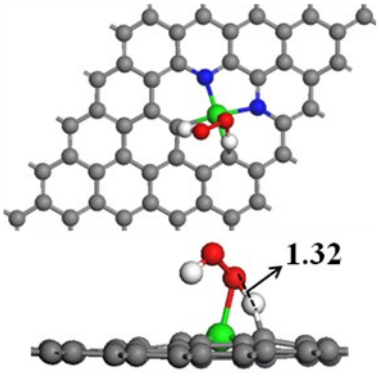


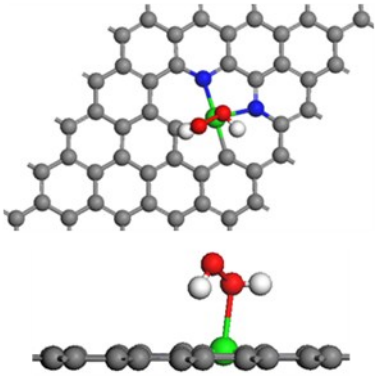




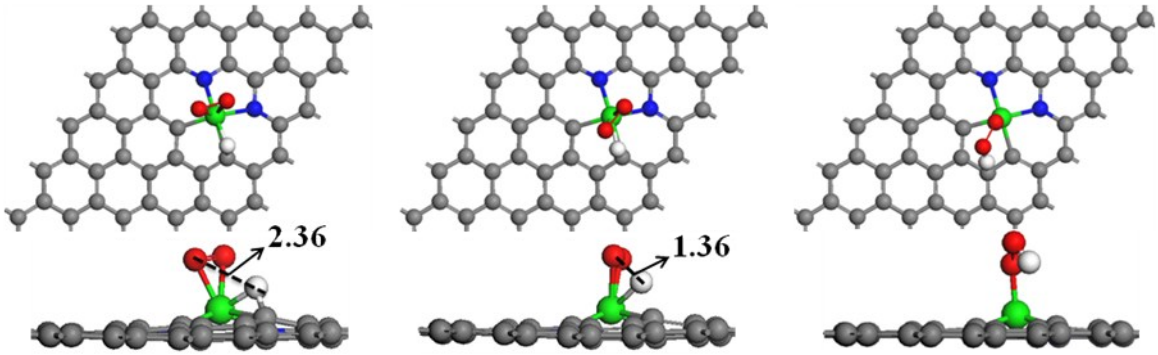
(b_3) *OOH + *H → *O + H_2O **ΔE = 0.22, ΔH = -2.62**







(b_5) *OOH + *H → *HOOH **ΔE = 0.70, ΔH = 0.19**



(a_2') *O_2+*H → *OOH **ΔE = 0.61, ΔH= -0.31**

Figure S2. Atomic structures of the initial state (left panel), transition state (middle panel), and final state (right panel) for reaction pathways on FeN_2-Gra. ΔE represents the energy barrier (eV) and ΔH represents the reaction energy (eV).