Supporting Information

DFT-based study on the mechanisms of the oxygen reduction reaction on Co(acetylacetonate)$_2$ supported by N-doped graphene nanoribbon

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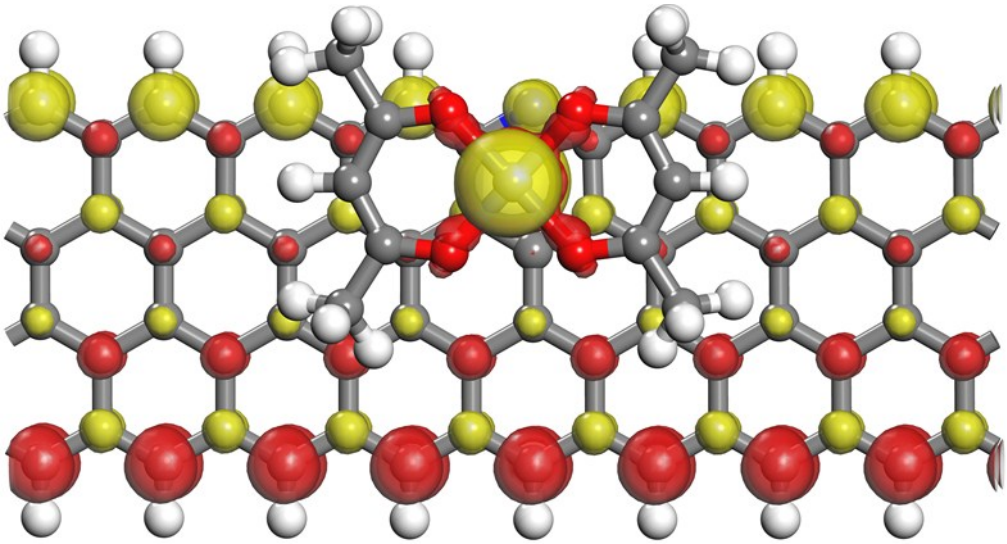
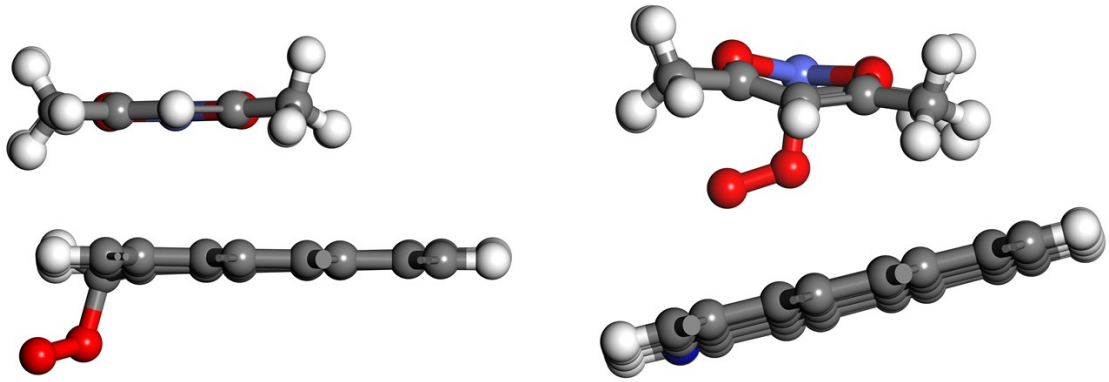


Fig. S1. The computed spin density of $Co(acac)_2$/N-doped graphene. The yellow and red denotes up- and down-spin states localized on opposite zigzag edges, and the isovalue is ±0.01 au.



(a) (b)

Fig. S2. The adsorption configurations of the O_2 molecule on (a) the outside surface of N-doped graphene, and (b) the interlayer of the $Co(acac)_2$/N-doped graphene nanoribbon,.

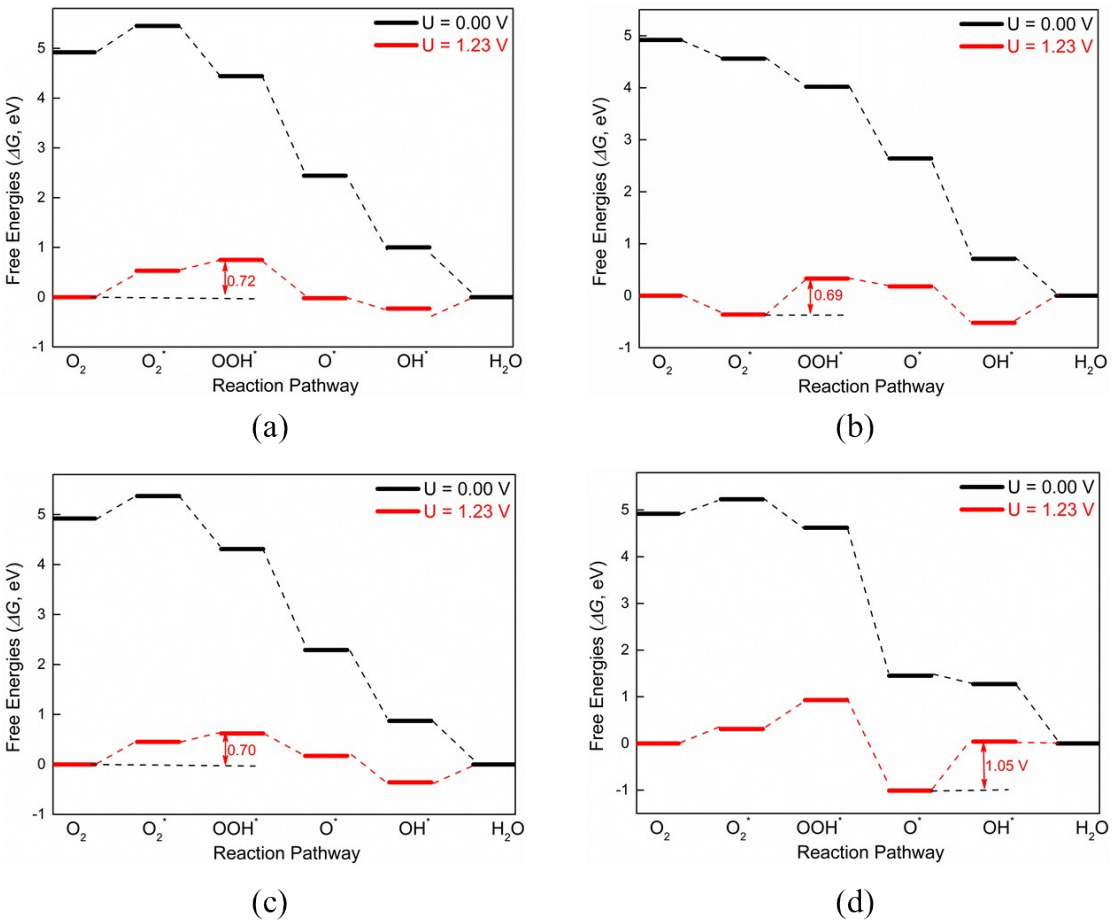


Fig. S3. The computed free-energy diagram of ORR on the (a) pristine N-doped graphene nanoribbon, (b) freestanding $Co(acac)_2$ complex, (c) outside surface of graphene, and (d) interlayer of the $Co(acac)_2$/N-doped graphene nanoribbon. Black and red lines represent reactions at zero electrode potential (U = 0 V) and the equilibrium potential (U = 1.23 V), respectively.