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Supporting Information

Single atom iron catalyst with single vacancy graphene-based substrate as a novel catalyst for NO oxidation: A theoretical study

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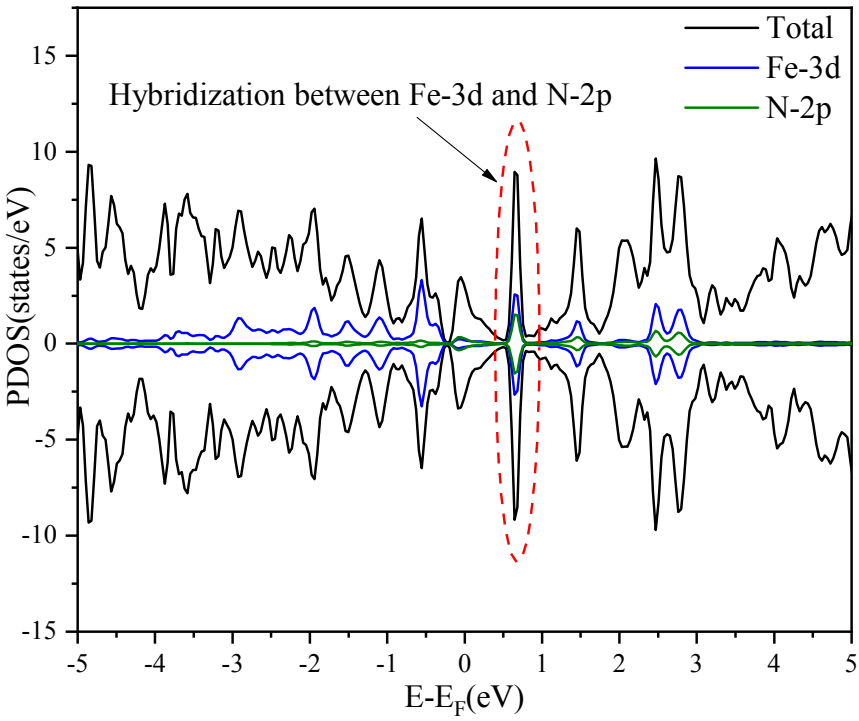
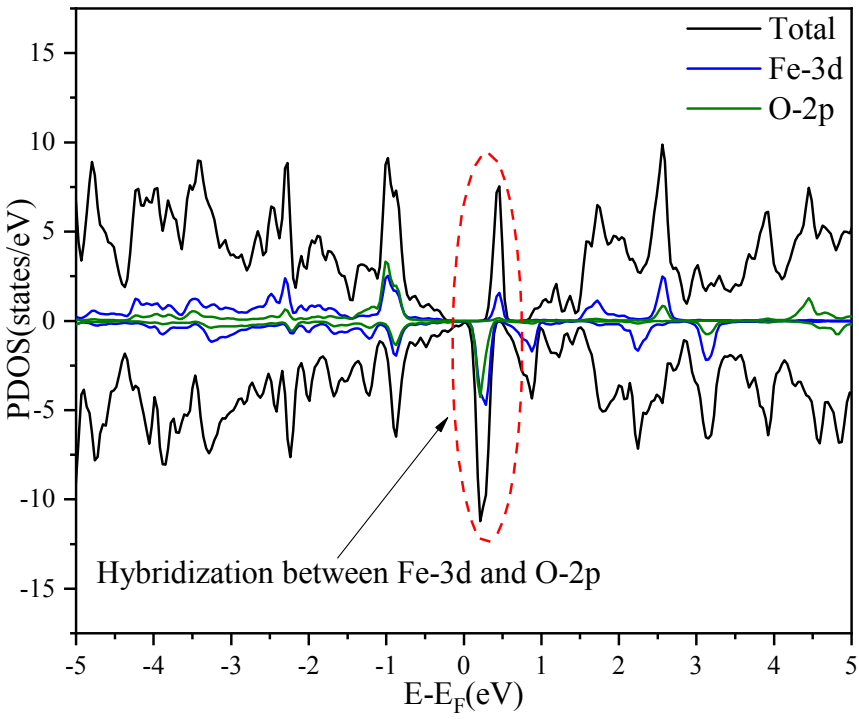

Total
Fe-3d
N-2p
Hybridization between Fe-3d and N-2p
PDOS(states/eV)
E-E$_F$(eV)

(a) NO


Total
Fe-3d
O-2p
Hybridization between Fe-3d and O-2p
PDOS(states/eV)
E-E$_F$(eV)

(b) O_2

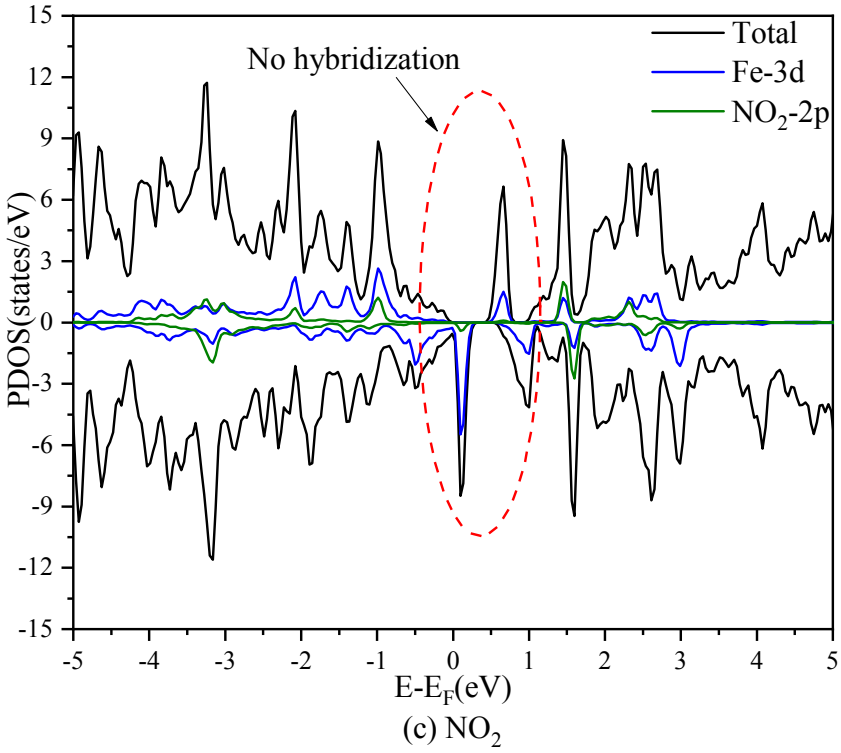


Fig. S1 The projected density of states of NO, O_2 and NO_2 adsorption configurations

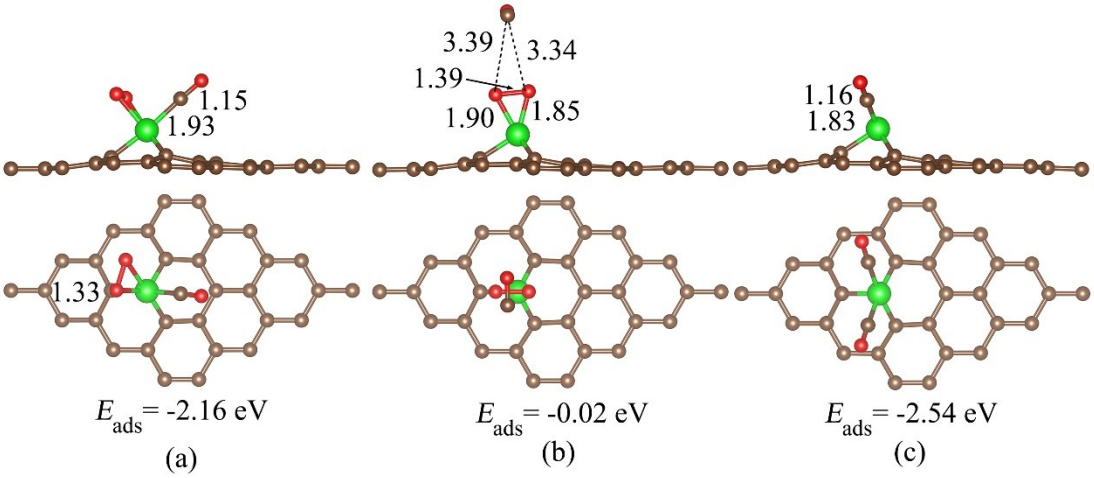


Fig. S2 The adsorption information of CO and O_2

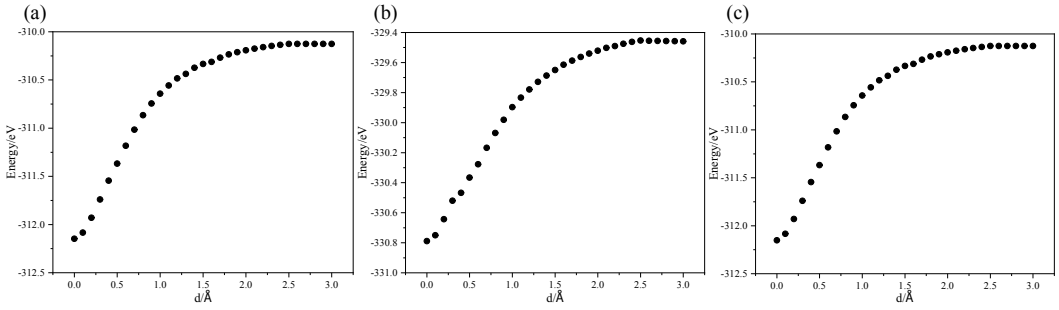


Fig. S3 The schemes of potential energy surface scanning ((a) is IM10, (b) is IM11, (c) is IM12)