Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electrocatalytic Oxygen Reduction Kinetics on Fe-center of Nitrogen-doped Graphene

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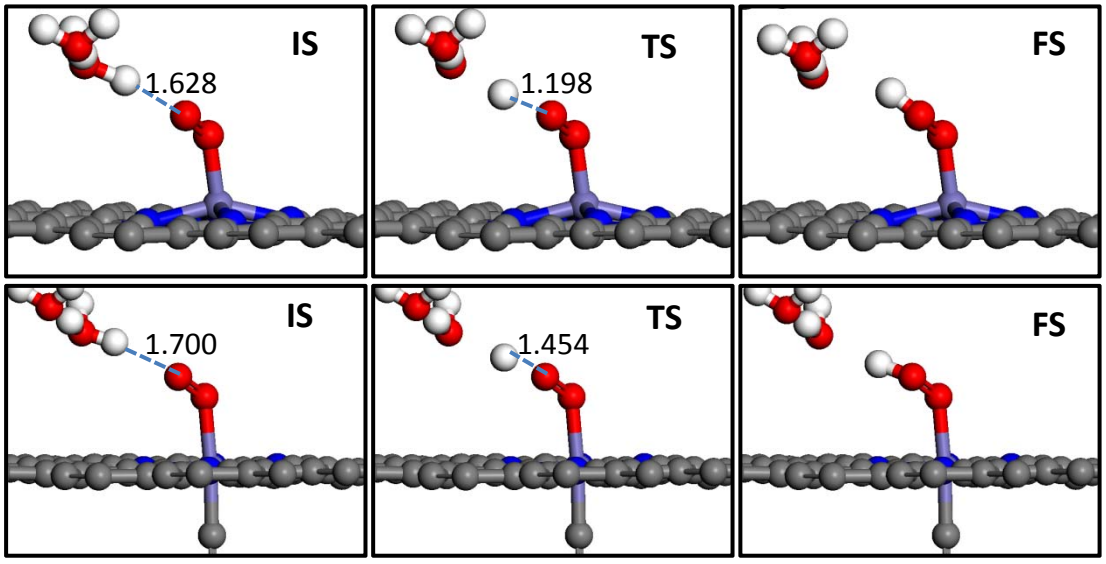

Figure S1. The IS, TS and FS structures of O_2 hydrogenation step. (O_2*+H^++e^-→OOH*) on FeN_4 (top panel) and $Fe(CN)N_4$ (bottom panel). The labeled distances are in angstroms. The grey, blue, red and purple balls represent C, N, O and Fe, respectively.

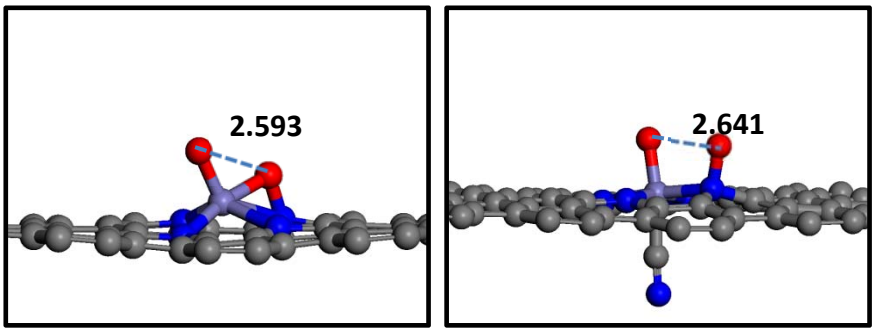

Figure S2 The dissociated O atoms on FeN_4 (Left) and on $Fe(CN)N_4$ (Right) at 0.8 V condition. The labeled distances are in angstroms. The grey, blue, red and purple balls represent C, N, O and Fe, respectively

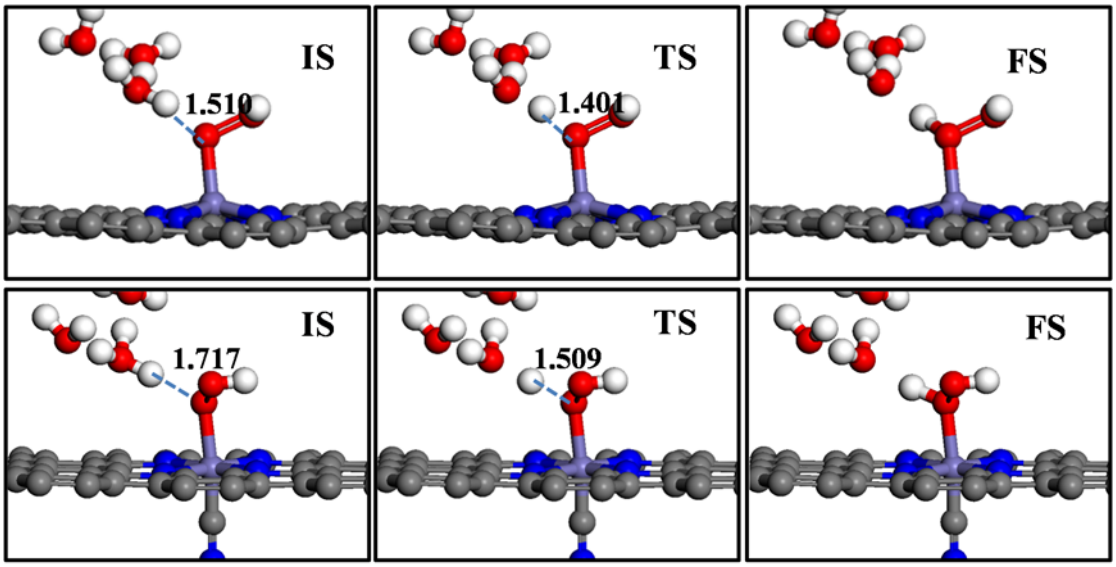

Figure S3. The IS, TS and FS structures for the OOH hydrogenation to H_2O_2 step ($OOH^*+H^++e^-\rightarrow HOOH^*$) on FeN_4 (top panel) and $Fe(CN)N_4$ (bottom panel). The labeled distances are in angstroms.

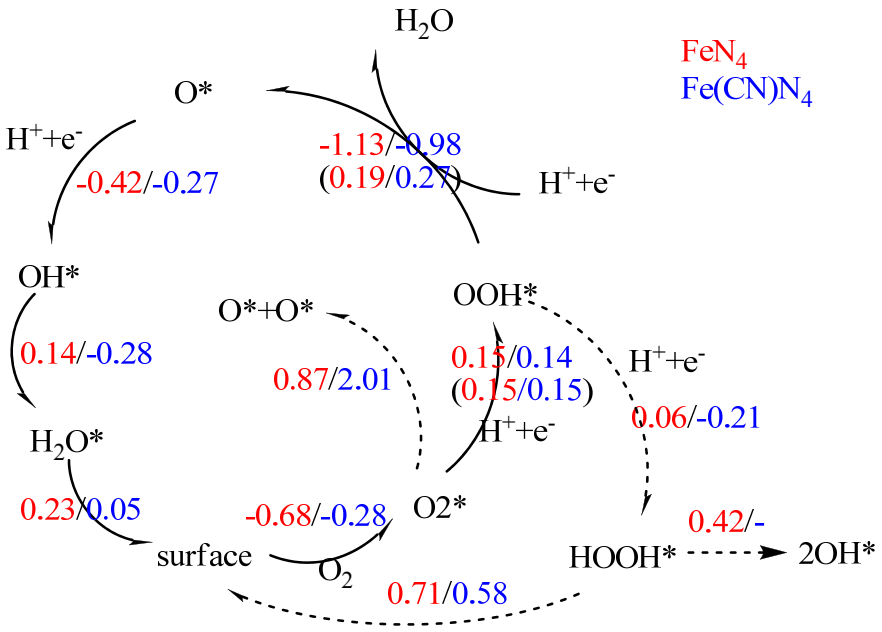

Figure S4: The complete mechanism of O_2 reduction on the two FeN sites. Indicated data are the free energy change of the reaction step at 0.8 V vs. SHE. The values in parentheses are the free energy barrier of the key elementary reactions. For the color of the data, Red represents FeN_4 site and blue for $Fe(CN)N_4$ site.