

Electronic supplementary information:

Graphyne-supported single Fe atom catalysts for CO oxidation

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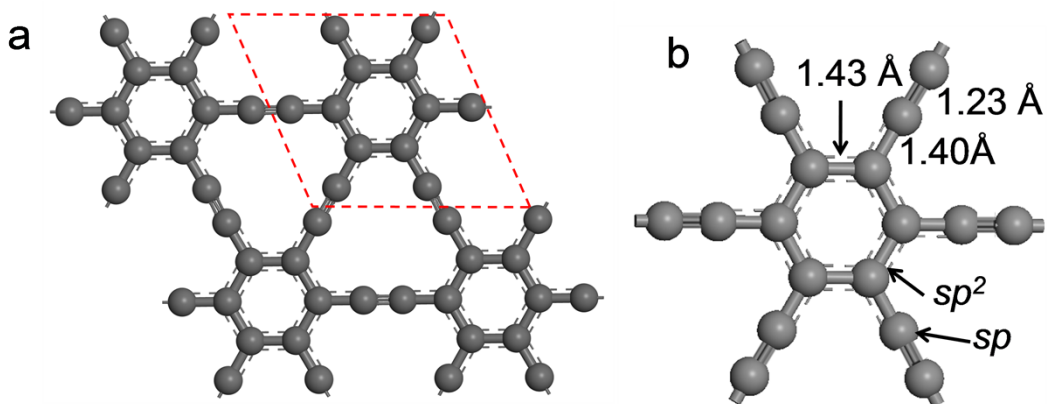


Fig. S1 (a) 2×2 supercells of the optimized graphyne single layer. The structure selected by dashed line represents primitive cell. (b) The primitive cell of graphyne.

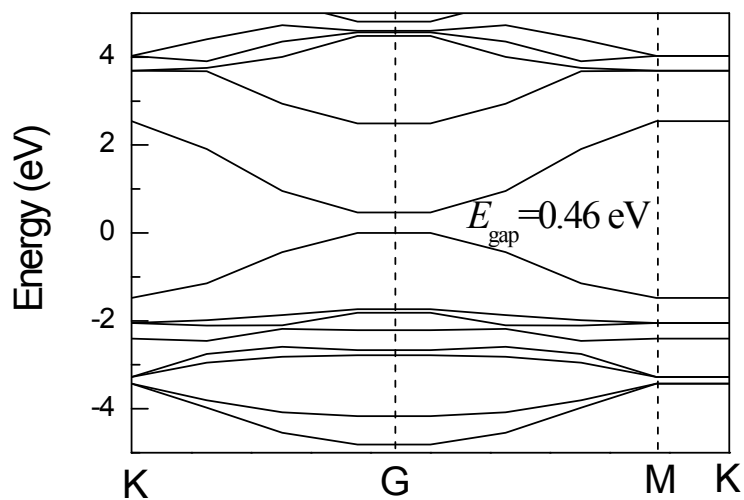


Fig. S2 Band structure of graphyne.

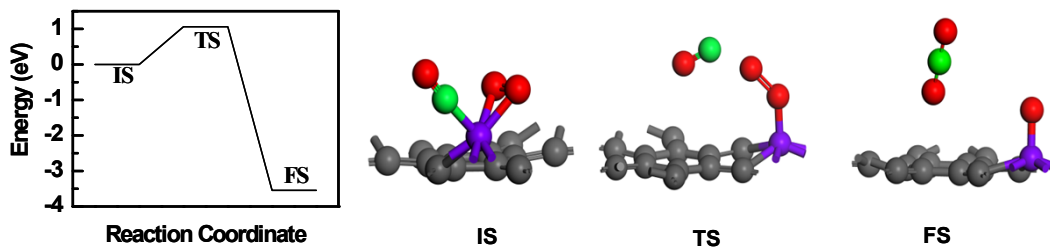


Fig. S3 Configurations of each state and minimum energy profiles for CO oxidation reaction on Fe-graphyne sheet along LH mechanism, including initial state (IS), transition state (TS), and final state (FS). Atomic color code: gray, carbon; red, oxygen.

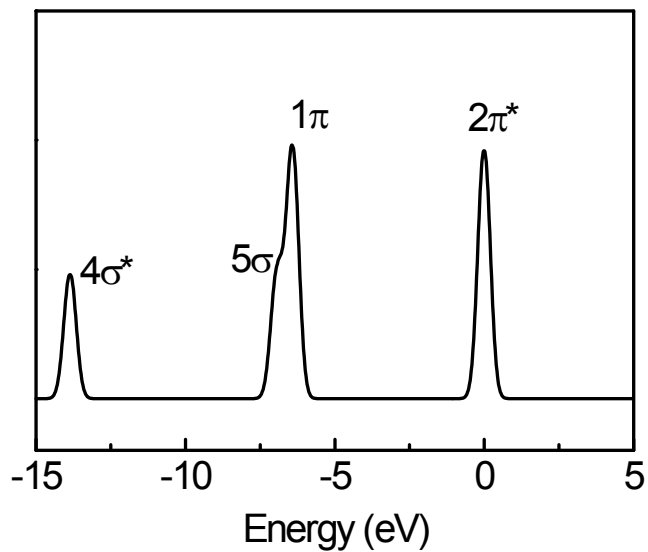


Fig. S4 LDOS of the isolated O₂ molecule.

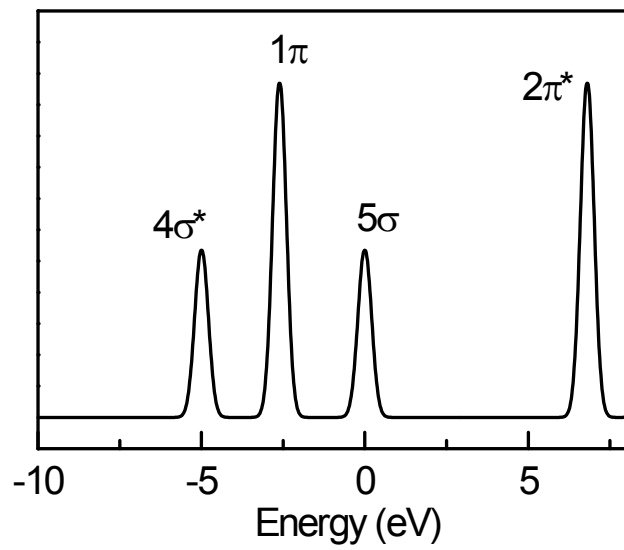


Fig. S5 LDOS of the isolated CO molecule.