Electronic supplementary information (ESI):

Graphdiyne as a metal-free catalyst for low-temperature CO oxidation

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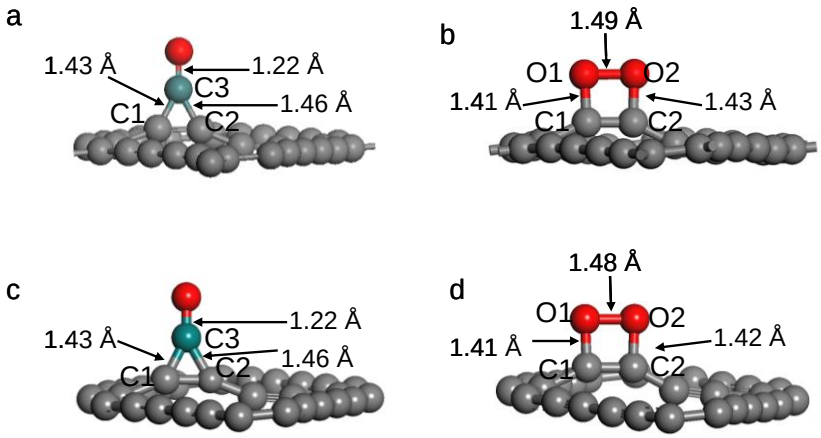

Fig. S1 Comparison of the configurations of the CO and O_2 adsorbed on graphdiyne surface obtained from CASTEP code (a, b) and DMol3 code (c, d).

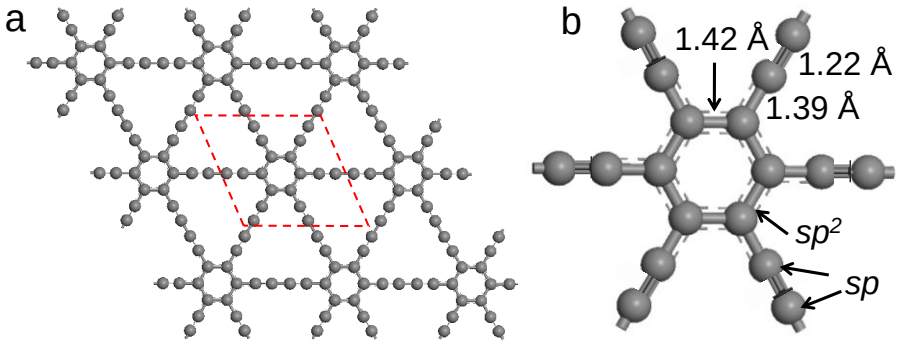

Fig. S2 (a) 3×3 supercells of the optimized graphdiyne single layer. The structure selected by dashed line represents primitive cell. (b) The primitive cell of the graphdiyne.

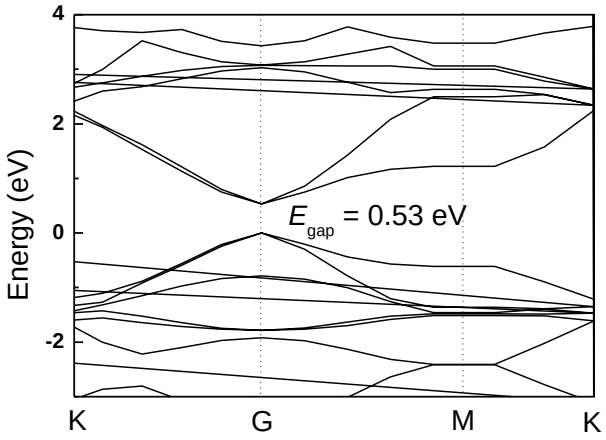

Fig. S3 Band structure of the graphdiyne.

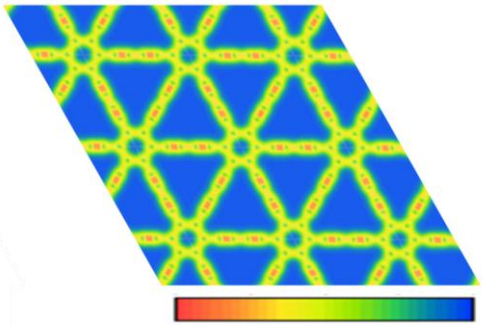

Fig. S4 Charge density plots of the 3×3 supercells of the graphdiyne. The red and blue colors represent positive and negative charges density, respectively.

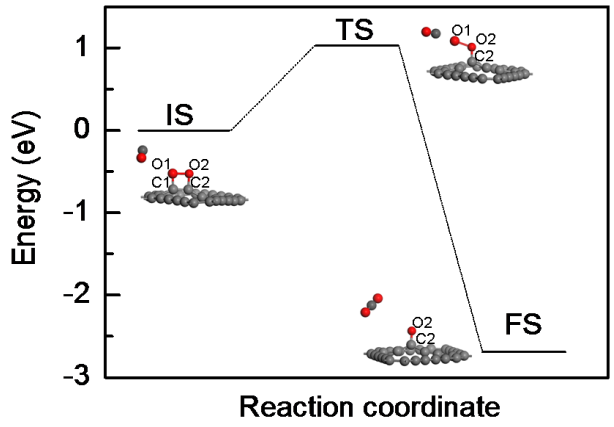

Fig. S5 Configurations of each state and minimum energy profiles for CO oxidation reaction on graphdiyne sheet along the LH mechanism, including initial state (IS), transition state (TS), and final state (FS). Atomic color code: gray, carbon; red, oxygen.

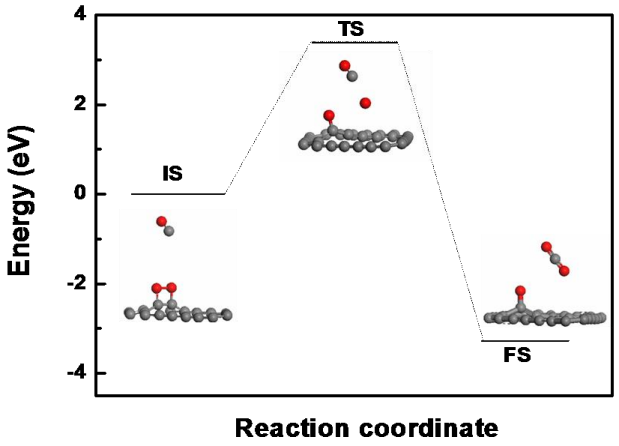

Fig. S6 Configurations of each state and minimum energy profiles for CO oxidation reaction on graphdiyne sheet along pathway I in ER mechanism, including initial state (IS), transition state (TS), and final state (FS). Atomic color code: gray, carbon; red, oxygen.