Electronic Supplementary Material (ESI) for RSC Advances.

A theoretical study of formaldehyde adsorption and decomposition on WC(0001) surface

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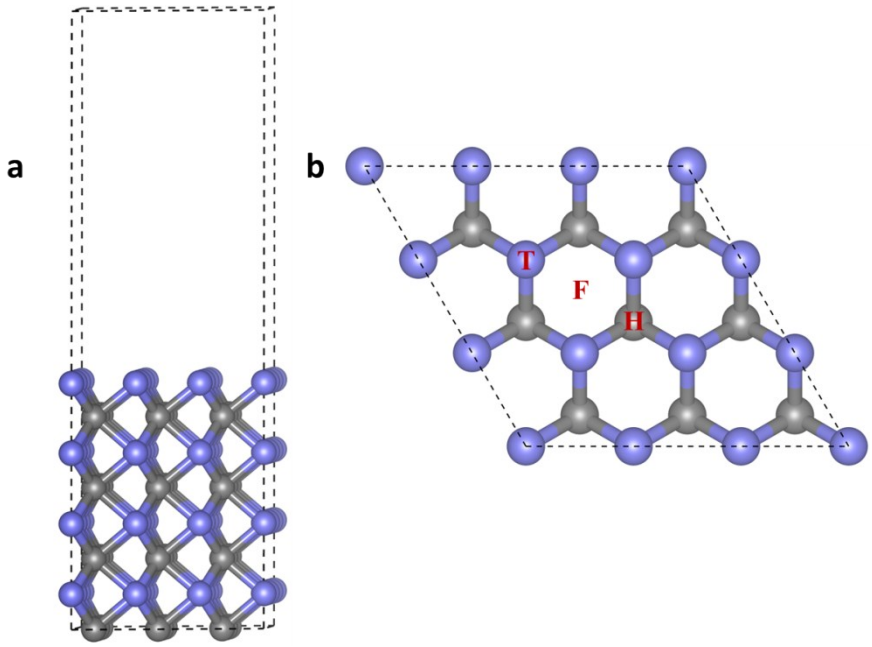

Figure S1 Optimized structure of clean WC (0001) surface: (a) side view, and (b) top view. Gray and blue balls represent C and W atoms, respectively. To analyze the adsorption, three sites with high symmetry were considered: top site (T), fcc site (H), and hcp site (H).

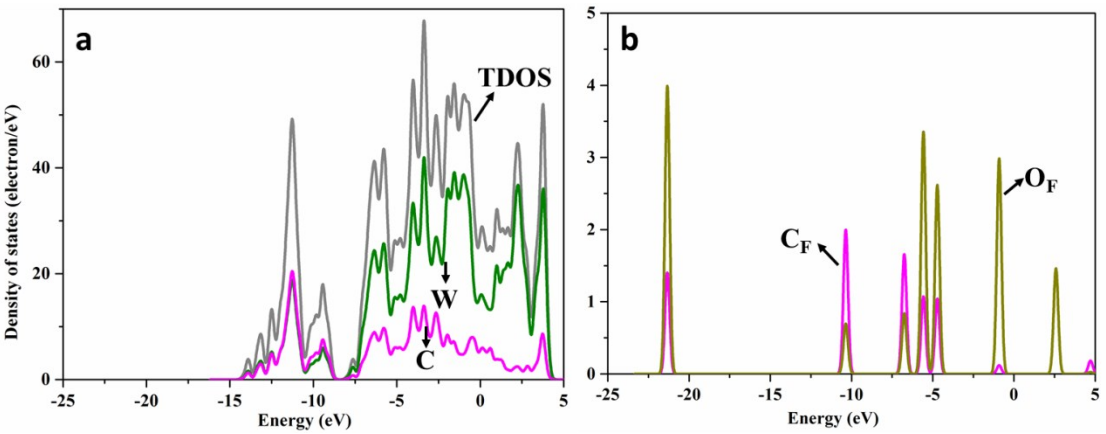

Figure S2 (a) DOS and PDOS of clean WC (0001) surface; (b) PDOS of HCHO molecule. The gray curves present TDOS for WC (0001) surface. PDOS of C, W and O atoms are denoted by pink, olive and dark yellow curves, respectively. The Fermi level of clean WC (0001) surface is assigned at 0 eV.

Table S1 The calculated adsorption energies at the most stable sites of various species produced in the process of HCHO decomposition.

Surface species	Adsorption energy (eV)
O	5.06
CO	1.17
CHO	3.88
CH_2	5.97
CH_3	3.52
C_2H_4	1.55
CH_4	0.01