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Sub-stoichiometric $WO_{2.9}$ for formaldehyde sensing and treatment: a first principles study

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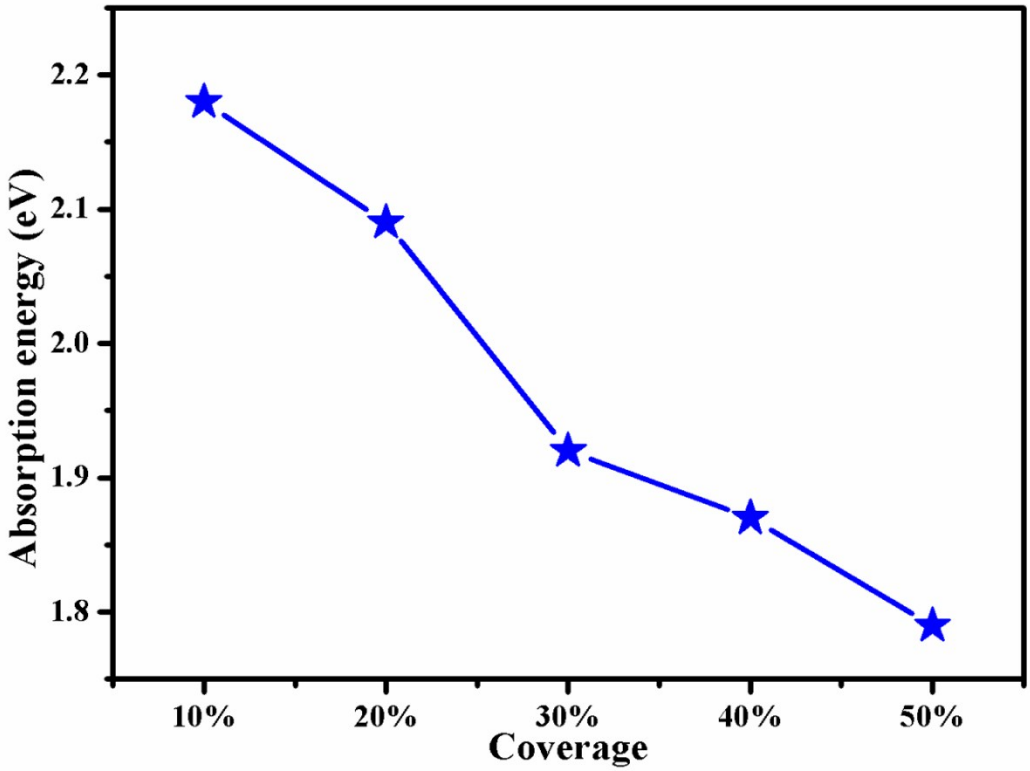

Figure S1. Coverage-dependent absorption energies of HCHO on WO2.9 (010) surface in configurations of type I.

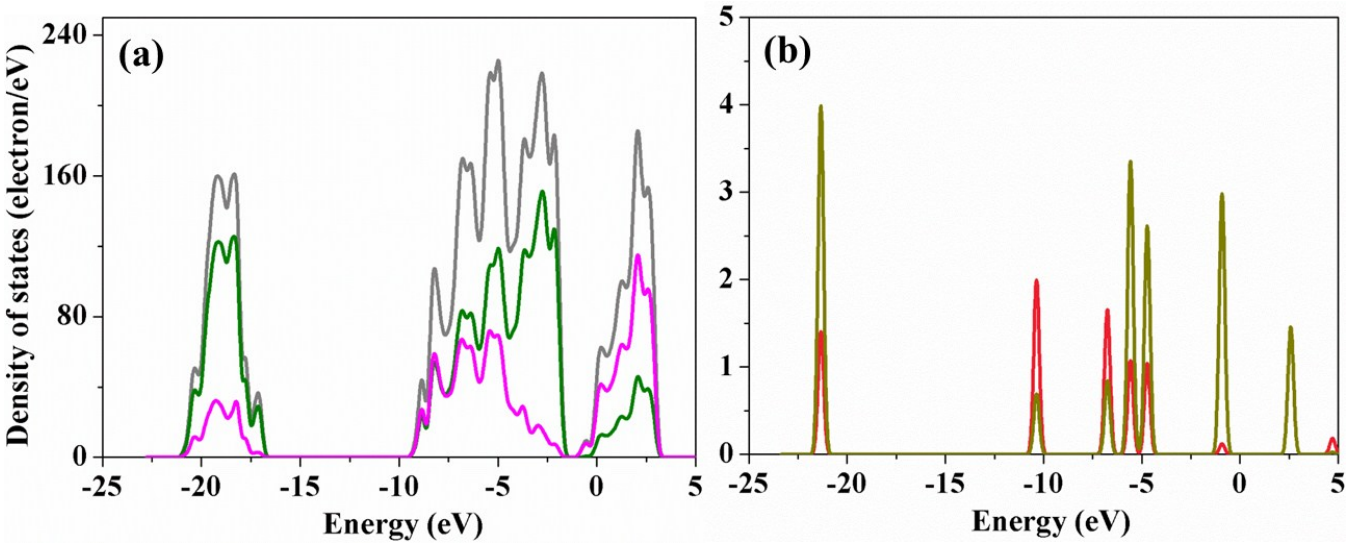

Figure S2. (a) The total density of states (TDOS) for $WO_{2.9}$ (010) surface (Gray curve) and DOS projected on the O atoms (Olive curve) and on the W atoms (Pink curve); (b) DOS projected (PDOS) on the C_F atom of HCHO molecule (Magenta curve) and on the O_F atom of HCHO molecule (Dark yellow curve). The Fermi level of $WO_{2.9}$ (010) surface is assigned at 0 eV.

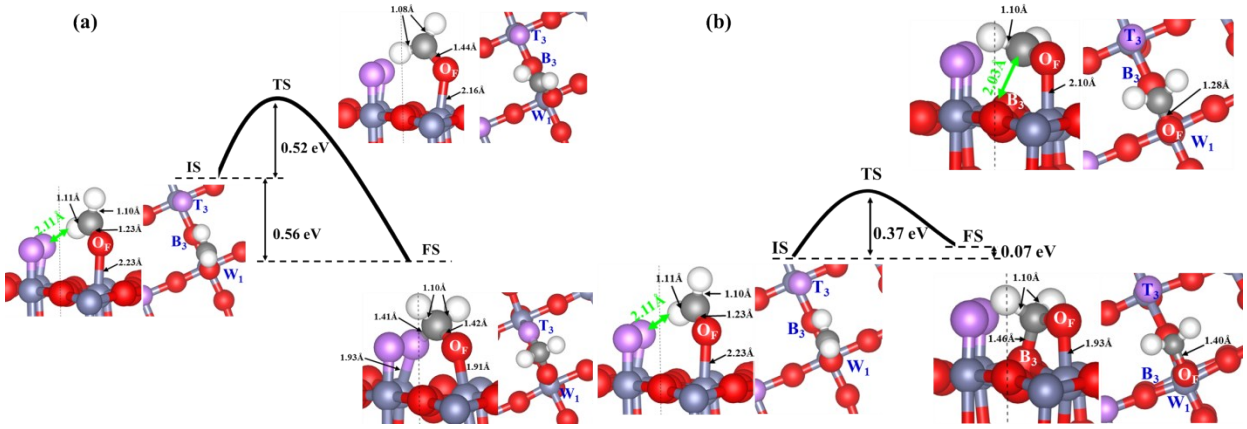

Figure S3. The barriers and the corresponding transition states of (a) the Type I and (b) the type III adsorption configurations transformed from type IV.

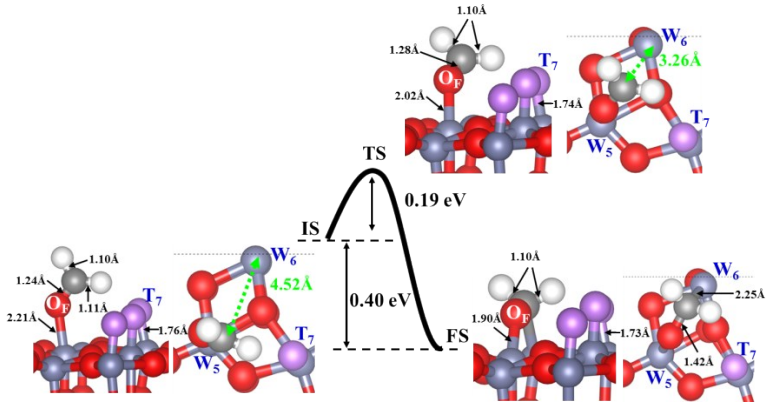

Figure S4. The minimum energy path for HCHO absorption configuration transform from type IV to type II.