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METHANOL FORMATION FROM SYNGAS ON ZnO (010) SURFACE: INSIGHTS FROM DFT

The synthesis of methanol from syngas ($CO/CO_2/H_2$) via hydrogenation on the ZnO (010) surface supported by CuPd cluster has been studied using periodic density functional theory (DFT) calculations. Our findings indicate that direct hydrogenation of CO_2 to methanol is selective. In the presence of surface atomic hydrogen and oxygen, CO_2 tends to form highly stable formate (HCOO) and formyl (HCO). Conversely, methanol production through CO hydrogenation is both thermodynamically and kinetically viable. CO undergoes successive hydrogenation steps, forming intermediates such as formyl (HCO), formaldehyde (H_2CO), and methoxy (H_3CO), ultimately yielding methanol (H_3COH). In the sequential hydrogenation of CO, the rate-limiting step is the conversion of methoxy (H_3CO) to methanol (H_3COH). Notably, the presence of CuPd cluster significantly promotes this final hydrogenation step, reducing the adsorption energy from -0.65 eV to -3.25 eV.

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