The influence of different supports on CO oxidative coupling to dimethyl oxalate

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ABSTRACT

CO oxidative coupling to DMO is an important step in the process of coal to ethylene glycol,[1] and Pd-based catalyst is the most effective catalyst.[2] However, the large-scale industrial production is greatly limited because of expensive price of Pd.[3] Noble metals dispersed on supports can not only reduce the amount, but also improve the catalytic activity of catalysts.

Density functional theory (DFT) was used to study the catalytic performance of Pd_6 loaded on α-Al_2O_3 (0001), TiO_2-O_v (001) and MgO-O_v (001) surfaces aiming at the oxidative coupling of CO. The results show that the $COOCH_3$-$COOCH_3$ coupling path is the favorable one on three catalysts, which is similar to that on the Pd(111) surface.[4]

The catalytic activity of three catalysts is compared with the Pd(111) surface,[4] and the order follows: Pd_6/α-Al_2O_3 > Pd_6/TiO_2-O_v > Pd(111) > Pd_6/MgO-O_v, as shown in Fig. 1. Therefore, Pd_6/α-Al_2O_3 has the highest catalytic activity, it is in good agreement with experiment that α-Al_2O_3 supported Pd catalyst has good catalytic activity for formation of DMO.[5] In addition, all of them display a good selectivity toward DMO.

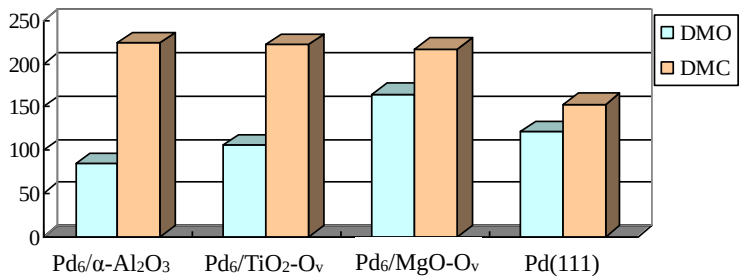

Fig. 1 Energy barriers of forming DMO and DMC during CO oxidative coupling on Pd_6/α-Al_2O_3, Pd_6/TiO_2-O_v and Pd_6/MgO-O_v catalysts.

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