Density functional theory studies of methanol steam reforming on PdZn and Cu

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Methanol steam reforming (MSR) is an attractive approach to on-board H_2 generation for fuel cells. To understand the mechanism of MSR on a new PdZn/ZnO catalyst, planewave density functional theory calculations are performed to explore the reaction pathways on the traditional catalyst Cu and the new PdZn catalyst. A network of reaction pathways have been identified for both catalysts, and they are quite similar. A key reaction in MSR is that between adsorbed formaldehyde (CH_2O*) and hydroxyl (OH*), which eventually leads to the CO_2 and H_2 products