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. Here, the reaction network on Cu(111) involving both formate (CHOO**) and methyl formate (CHOOCH3*) is shown with activation energies, reaction energies, as well as adsorption energies. A similar network is operative on PdZn(111).