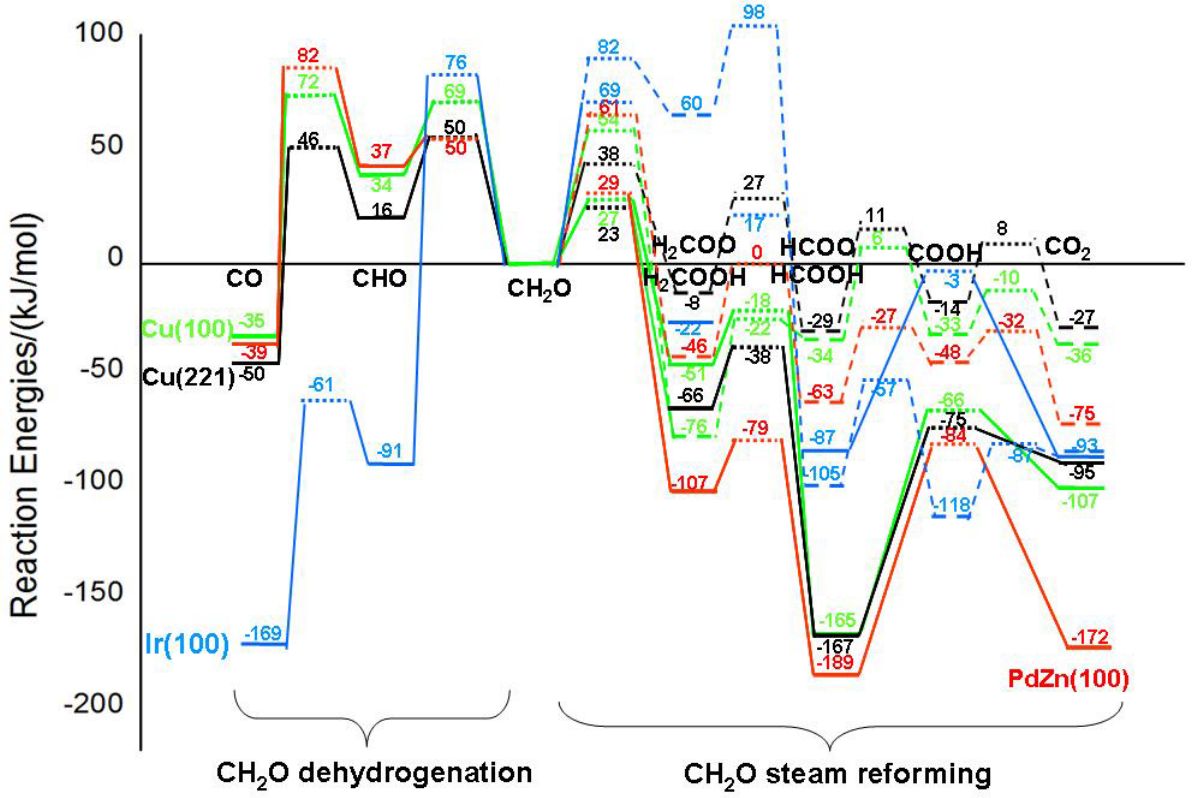
Formaldehyde Steam Reforming on Cu, PdZn and Ir

Density functional theory has been used in this study to investigate the steam reforming of formaldehyde and its reaction intermediates on Cu (221), PdZn (100) and Ir (100) surfaces. The adsorption complexes (CH_2O, H_2COOH, H_2COO, HCOO, COOH, etc.), binding energies and reaction energies involved in the steam reforming and dehydrogenation of formaldehyde have been systematically characterized. Our results showed that CH_2O dehydrogenation is the dominant pathway for Ir(100). In contrast, desorption of CH_2O is more favorable on regular Cu and PdZn (100) surfaces compared to dehydrogenation and the steam reforming reaction is likely to occur at defect site such as Cu(221) surface.

K. H. Lim*, *ChemCatChem* **2012**, In press.



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