

Interaction of Methanol and Its Dehydrogenation Species with Pt-alloy Surfaces

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First Author	Cahyanto, Wahyu Tri; Widanarto, Wahyu; Effendi, Mukhtar;
Last Author	Kasai, Hideaki
Authors	Cahyanto, WT; Widanarto, W; Effendi, M; Hamdi, MR; Kasai, H;
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Abstract	Adsorption of sequential single methanol dehydrogenation intermediate species on Pt-, PtRu-, and PtRuMo-surfaces is investigated by using density functional theory (DFT). This work is a part of our efforts in understanding the methanol oxidation reaction (MOR) on Pt- alloy surfaces for further possible prediction of decomposition processes. Particularly, effects of Ru and Mo impurity to the pure Pt surface to form PtRu and PtRuMo surfaces as possible candidates for promising catalysts of direct methanol fuel cells (DMFCs) are given. However, the study is limited to the scientific point of view, i.e., fundamental interactions between adsorbates and surfaces, in correspondence with adsorption mechanism using charge transfer analysis. The trend in the increase of adsorption energy and charge transfer by alloying Ru and Mo to the Pt surface is observed. Moreover, the increase of the d-orbital vacancy caused by alloying Ru and Mo possessing lesser filled d-orbital is suggested to responsible for the increase of surface-adsorbate interaction strength.
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Author	WAHYU TRI CAHYANTO, S.Si, M.Si, Ph.D