Adsorption of formaldehyde and formyl intermediates on Pt, PtRu-, and PtRuMo-alloy surfaces: A density functional study

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Abstract	Stable binding configuration for formaldehyde (H2CO) and formyl (HCO) adsorption on Pt, PtRu, and PtRuMo are studied within the frame of density functional theory (DFT). We address this study to investigate the role of Ru and Mo on the binding characteristic of formaldehyde and formyl adsorption with respect to interaction strength and charge analysis. Several binding conformation on all possible surface adsorption sites are considered in determining the most stable adsorption geometry on three surfaces. Our results show that the presence of Ru in PtRu and Mo in PtRuMo stabilize the formaldehyde and formyl, which are indicated by stronger bond strength. Further electronic structure analysis shows that the addition of Ru in PtRu and Mo in PtRuMo modifies the electronic structure of Pt's surface significantly. The presence of both impurities shifted the derived anti-bonding state - which is originally located below the fermi level in pure Pt surface - to be above the fermi level in PtRu and PtRuMo systems. This fact explains the stronger adsorption found on PtRu & PtRuMo as compared to pure Pt surface. (C) 2012 Elsevier B.V. All rights reserved.
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