Theoretical studies of the adsorption of hydroxymethylidyne (COH) on Pt-alloy surfaces using density functional theory

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Abstract	We present density functional calculations for the adsorption of hydroxymethylidyne (COH) on Pt, PtRu, and PtRuMo (111) surfaces. Here we clarify the adsorption mechanism by using a charge transfer analysis related to the adsorption energy. We observe that the preferred binding sites for COH are the hcp hollow Pt-Pt-Pt, hcp hollow Pt-Ru-Pt, and hcp hollow Pt-Ru-Pt adsorption sites for Pt, PtRu, and PtRuMo, respectively. Addition of Ru to form a PtRu surface increases the adsorption energy, while addition of Mo to form a PtRuMo surface decreases it. Our analyses show that the adsorption energy is determined by electron transfer between the molecular COH and the metal surfaces associated with bonding.
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