Preferential sites for adsorption of methanol and methoxy on Pt and Pt-alloy surfaces

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Abstract	We studied the site preference of methanol (CH(3)OH) and methoxy (CH(3)O) on Pt, PtRu and PtRuMo surfaces using density functional theory. This work aimed to investigate the nature of methanol and methoxy adsorption in relation to energetic properties and charge transfers and to clarify the role of alloying metal Ru and Mo on adsorption properties. Similar adsorption geometry of methanol and methoxy on these three surfaces was observed. The largest charge transfer was observed on methanol and methoxy adsorption on PtRuMo-, followed by PtRu- and Pt-surfaces, resulting in the strength order of binding energy. We also found that Mo in PtRuMo donates the largest amount of charge, followed by Ru in PtRu and Pt in the pure Pt surface; we concluded that this is responsible for the preferential adsorption sites of methanol and methoxy.
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