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Structural Investigation of Binary Palladium-Gallium Alloys with In Situ XAS

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Palladium is an important catalyst for hydrogenation and for combustion reactions. The binary alloys PdGa and Pd₃Ga₇ are stoichiometric compounds with ordered structures. These materials are particularly interesting as possible catalysts due to isolation of the Pd atoms in the structure. In both structures the Pd atoms are surrounded by a closed coordination sphere of Ga atoms (i.e. coordination number of 7 in PdGa and of 8 in Pd₃Ga₇). Conversely a supported Pd catalyst presents an ensemble of neighboring Pd-atoms to the reactants. This significant difference in structures between Pd metal and the alloys may provide a unique selectivity. Here, we present results from in situ XAS measurements designed to determine the thermal stability of these alloys in the presence of various gas atmospheres. We determined the behavior of the bulk alloys in helium, 5% hydrogen, and 20% oxygen, as well as in the catalytically interesting mixtures of CO and oxygen, and propene and hydrogen at temperatures from 293 to 773 K. First results show an unexpectedly high stability in either highly reducing or highly oxidizing atmospheres. Additionally, both compounds show a moderate catalytic activity for propene hydrogenation and a slight catalytic activity for CO oxidation. Results of our XAS investigation of both the Pd and the Ga K edges will be presented with complimentary data from in situ XRD and thermal analysis.