356d Promotional Effect of Fe on the Wgs Activity of Pd and Pt Based Catalysts

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This study describes the effect of Fe on Pd and Pt catalysts on the low temperature Water Gas Shift (WGS) reaction. We have successfully prepared Fe alloys with Pt or Pd. Mössbauer and XRD show that under reducing conditions alloys (PdFe or Pt_3Fe) and α-Fe coexist. On exposing the catalysts to water gas shift conditions, some iron gets oxidized to Fe_3O_4 whereas some remains in the alloy phase. The kinetics of the water gas shift reaction shows that Fe has a significant promotional effect on the WGS activity of both Pd and Pt catalysts; the effect is more pronounced with Pd than with Pt. From experiments alone, it is difficult to determine which of the two phases is responsible for the enhanced activity. Self-consistent, periodic DFT calculations on a variety of model systems are used to elucidate the reasons for the observed enhanced WGS activity.