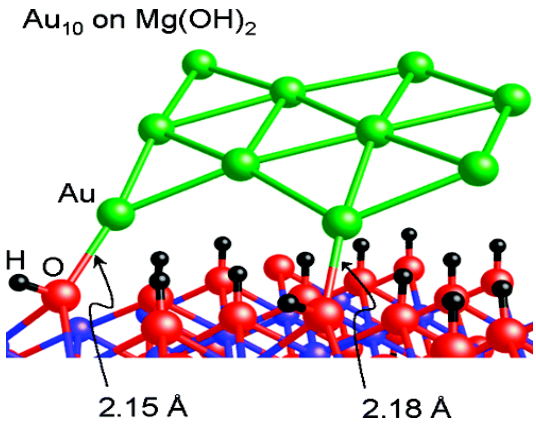
Enhanced metal-support interactions for more stable catalysts

Computational studies have now provided a clear picture of how gold nanoclusters interact with surface hydroxyls, ubiquitous to all oxide surfaces, and how these hydroxyls enhance catalyst stability. By using a density functional theory-enabled local basin-hopping technique for global-minimum search, researchers have found strong interactions between gold nanoclusters and hydroxylated supports. These interactions help prevent sintering of the gold nanoclusters, thereby stabilizing their high activity for carbon monoxide oxidation at low temperatures. Computational studies reveal that the gold cluster bonds to the support surface by forming multiple covalent anchors through the hydroxyl groups. For a $Mg(OH)_2$ support, each Au–OH bond enhances the stability by 0.8eV. Charge analysis indicates that the interfacial gold atoms are slightly positively charged, but the whole gold cluster has a partial negative charge, which could help adsorb carbon monoxide and catalyze its oxidation. This strong interaction is expected to be ubiquitous on hydroxylated support surfaces and it limits migration and aggregation of the gold nanoclusters. The effect of the interfacial structure on catalysis is now being explored. By *understanding the factors that control bonding of metal clusters on oxide supports, new catalysts with higher stability and better catalytic performance will be discovered.*



De-en Jiang, Steven H. Overbury and Sheng Dai Interaction of Gold Clusters with a Hydroxylated Surface. *J. Phys. Chem. Lett.* **2011**, *2*, 1211–1215