Catalysis by Gold

Duncan John Mowbray

Nano-Bio Spectroscopy Group and ETSF Scientific Development Centre
Departamento de Física de Materiales
Universidad del País Vasco, UPV/EHU and DIPC, Donostia-San Sebastián, Spain

Gold is the noblest of metals, and does not oxidize. This is because molecular oxygen both binds very weakly and fails to dissociate on gold. However, at the nanoscale gold can be extremely active for oxidation under mild conditions, e.g. $CO + 1/2\ O_2 \rightarrow CO_2$. This suggests that gold nanoparticles could be used to perform oxidation delicately, e.g. $CH_4 + 1/2\ O_2 \rightarrow CH_3OH$ or $CH_2O + H_2$. By employing density functional theory (DFT) calculations in a microkinetic model, we obtain a quantitative description of CO and H oxidation by O_2 and N_2O on gold nanoparticles.[1] However, modelling methane oxidation on gold nanoparticles is significantly more difficult. Although methane oxidation to CO2 has been observed experimentally, from DFT calculations we find neither CH_4, CH_3, nor H bind to a neutral gold nanoparticle. Further, the measured activation barrier shows a strong dependence on the nanoparticle's size. We will explore two possible reasons for the observed behaviour: charging of the gold nanoparticles, and melting to form gold dimers.

---

[1]Walther, G.; Mowbray, D. J.; Jiang, T.; Jones, G.; Jensen, S.; Quaade, U. J.; Horch, S. *J. Catal.* **260**, 86-92 (2008).