Electrocatalytic activity of bimetallic platinum-gold catalysts fabricated based on nanoporous gold

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1. Methanol oxidation at NPG electrode in acidic solutions

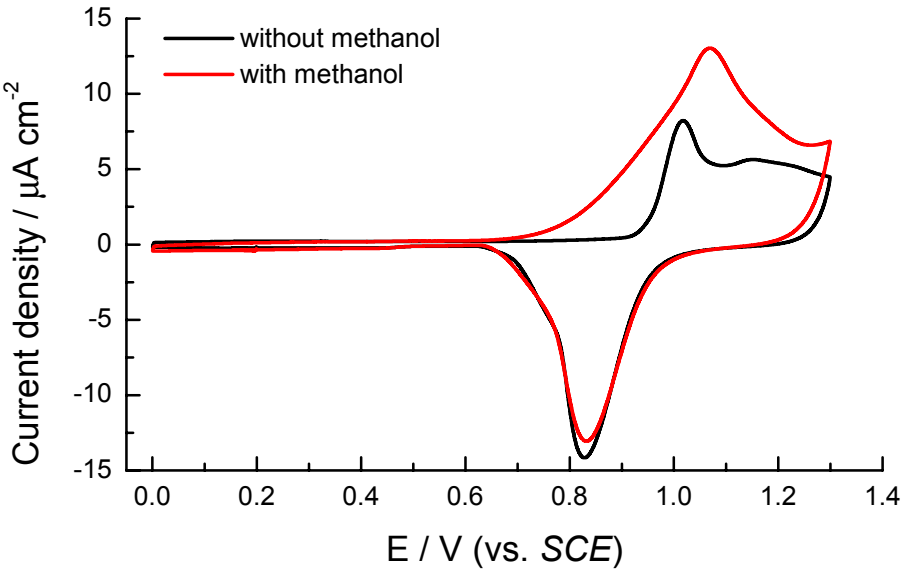
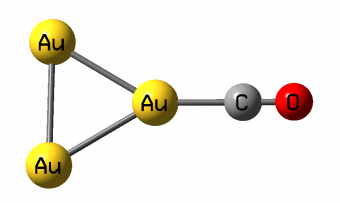


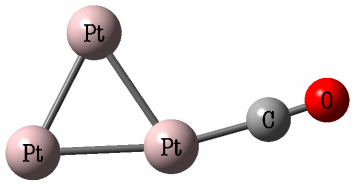
Fig.S1. The CVs of nanoporous gold (NPG) electrode in 0.1 mol dm^{-3} $HClO_4$ solution with and without 1.0 mol dm^{-3} methanol. Scan rate: 20 mV s^{-1}.

2. Theoretical calculation of CO or OH adsorption on bimetallic Pt-Au catalysts



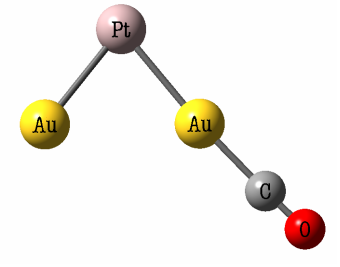
Au_3CO

(1.07)



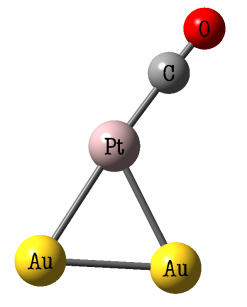
Pt_3CO

(2.00)



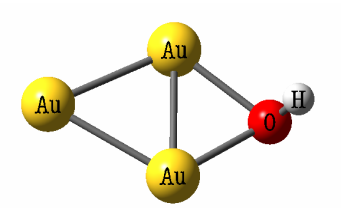
Au_2PtCO (I)

(1.21)



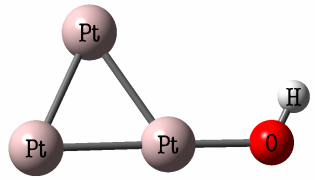
Au_2PtCO (II)

(2.38)



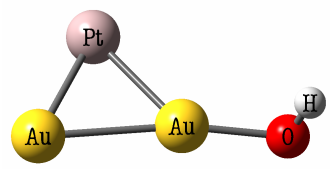
Au_3OH

(1.81)



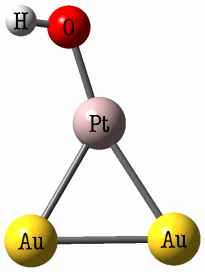
Pt_3OH

(2.62)



Au_2PtOH (I)

(1.81)



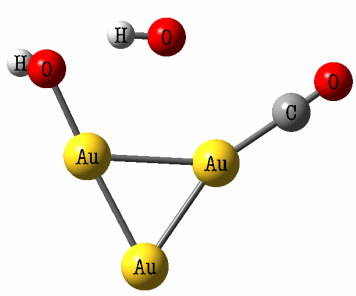
Au_2PtOH (II)

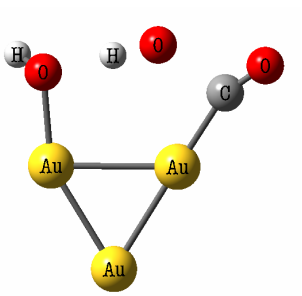
(2.48)

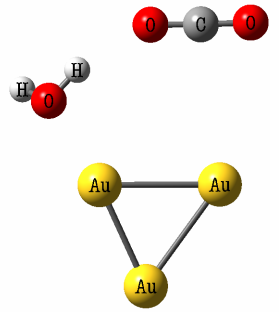
Fig.S2. Optimized configurations of CO and OH bound to the pure and binary trimers. The values given in parentheses are binding energies (in eV). The density functional theory (DFT) calculation was performed by means of the Gaussian 03 suite of programs.

3. Theoretical simulation of surface reaction between adsorbed CO and OH species on pure Au and bimetallic Pt-Au Catalysts

(a)



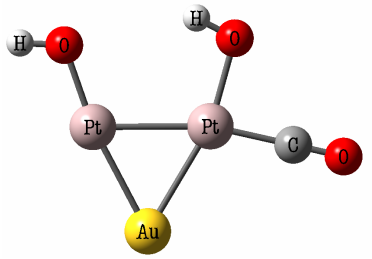


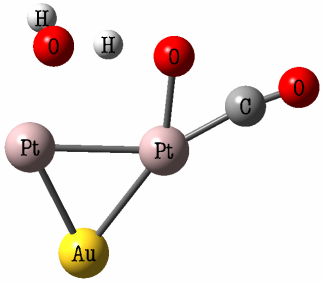


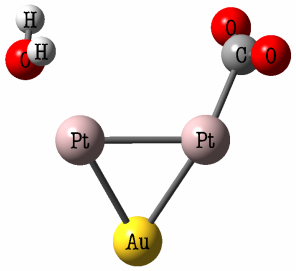
Total energy: (-671.418246 a.u.) (-671.406374 a.u.) (-671.510928 a.u.)

Relative energy: (0.0 kcal mol^{-1}) (7.45 kcal mol^{-1}) (-58.16 kcal mol^{-1})

(b)







Total energy: (-638.848825 a.u.) (-638.786696 a.u.) (-638.867662 a.u.)

Relative energy: (0.0 kcal mol^{-1}) (38.99 kcal mol^{-1}) (-11.82 kcal mol^{-1})

Fig.S3. The changes in potential energy for the reaction $2OH + CO=CO_2 + H_2O$ over pure Au trimer (a) and Pt_2Au binary trimer (b). The total energy of the isolated reactants is taken as the zero point.

4. Methanol oxidation at bulk Pt electrode in acidic solutions

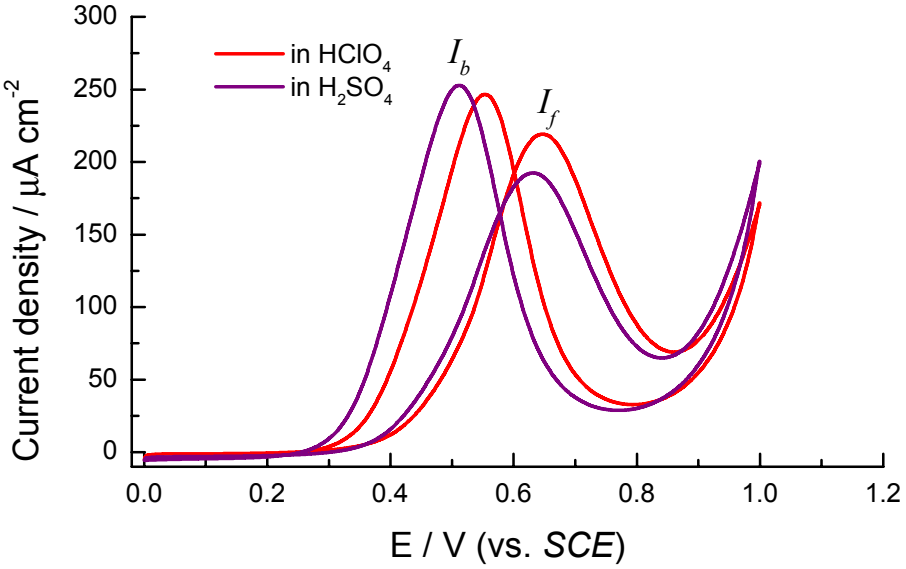


Fig.S3. CVs of the electro-oxidation of methanol (1.0 mol dm^{-3}) at a poly-crystalline platinum in 1.0 mol dm^{-3} $HClO_4$ or 0.5 mol dm^{-3} H_2SO_4 at 10 mV s^{-1}.

5. Electrooxidation of formic acid at NPG and NPG-Pt electrodes

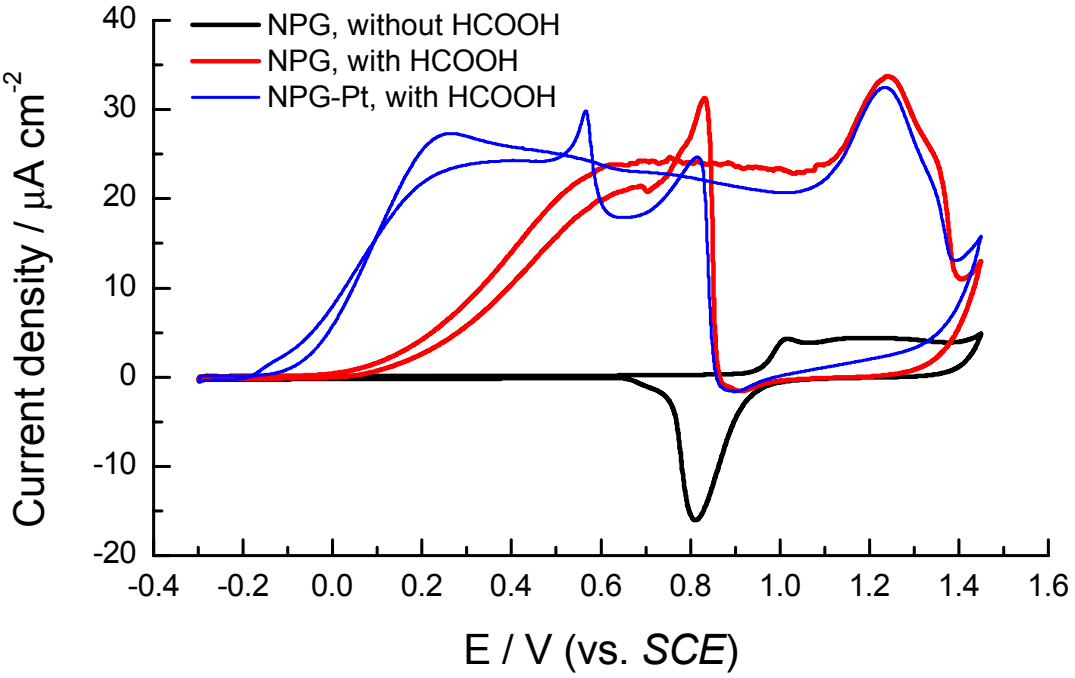


Fig.S4. CVs of the NPG and NPG-Pt electrodes in 0.1 mol dm^{-3} $HClO_4$ solutions with and without 0.2 mol dm^{-3} formic acid. The CVs of unmodified NPG electrode in 0.1 mol dm^{-3} $HClO_4$ was also superimposed on the figure as a contrast test. Scan rate: 10 mV s^{-1}.