Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Origin of high activity but low CO_2 selectivity on binary PtSn in the direct ethanol fuel cell†

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Supporting Information

Cyclic voltammograms of Pt and PtSn electrodes in the presence of ethanol at 60 °C (Figs. S1-3), phase diagram of OH adsorption on Pt(211) and Sn/Pt(211) (Fig. S4), energy profiles of ethanol adsorption and electrooxidation on Pt(211) (Fig. S5), optimized structures and located transition states during the ethanol adsorption and electrooxidation on Pt(211) (Fig. S6). See DOI: 10.1039/b000000x/

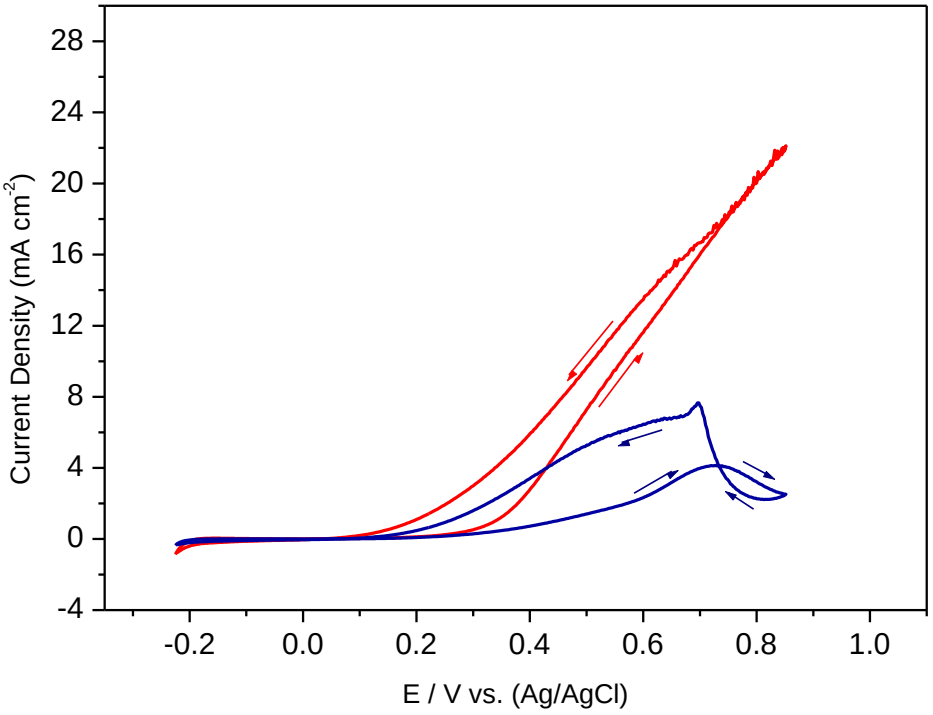

Figure S1. Cyclic voltammograms of the polycrystalline Pt in 2 M EtOH + 0.1 M H_2SO_4 at 20 ^oC (blue) and 60 ^oC (red). Scan rate 0.200 V s^{-1}.

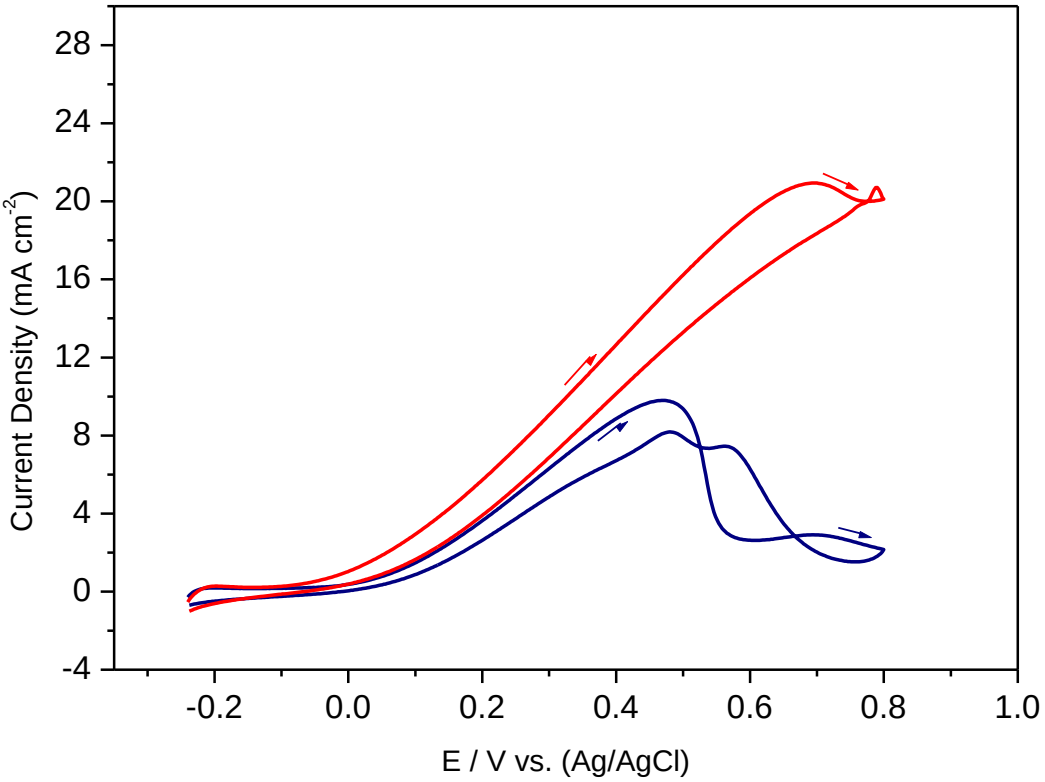

Figure S2. Cyclic voltammograms of the polycrystalline PtSn in 2 M EtOH + 0.1 M H_2SO_4 at 20 ^oC (blue) and 60 ^oC (red). Scan rate 0.200 V s^{-1}.

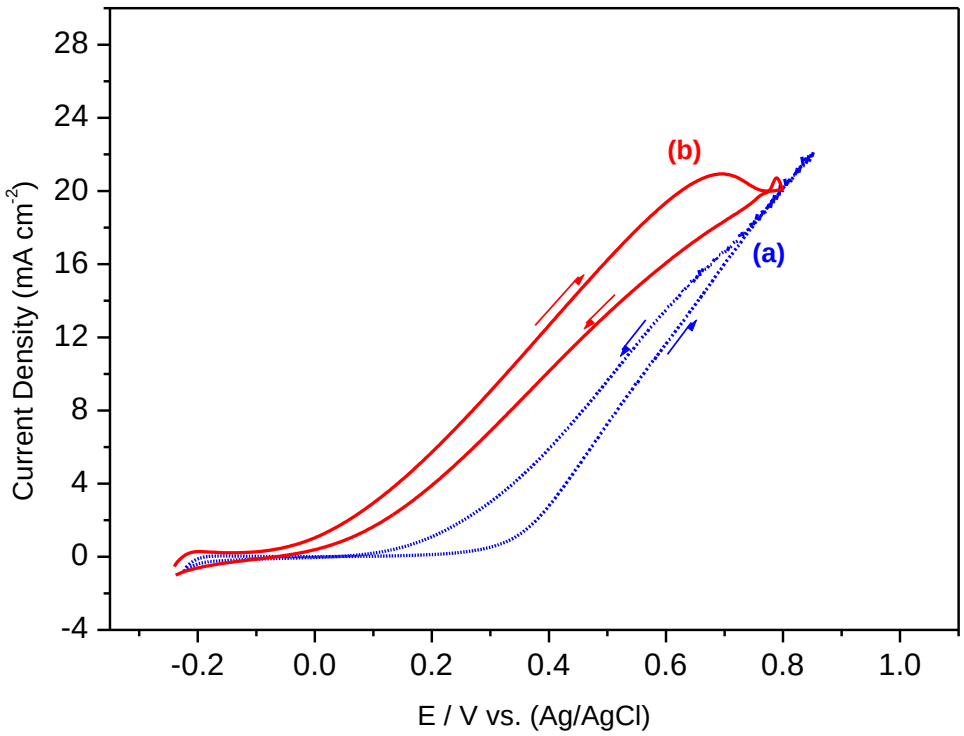

Figure S3. Cyclic voltammograms of the polycrystalline Pt (blue) and PtSn (red) in 2 M EtOH + 0.1 M H_2SO_4 at 60 ^oC. Scan rate 0.200 V s^{-1}.

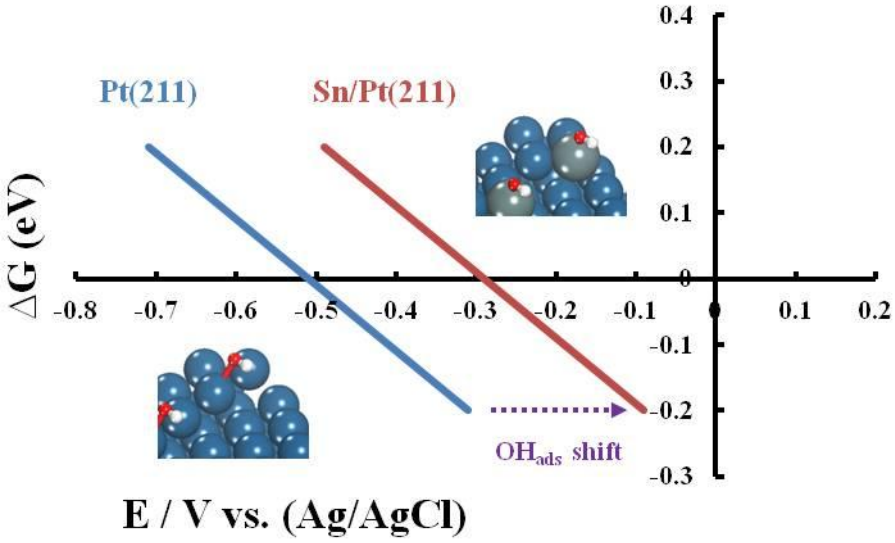

Figure S4. Calculated phase diagram of OH adsorption on Pt(211) and Sn/Pt(211).

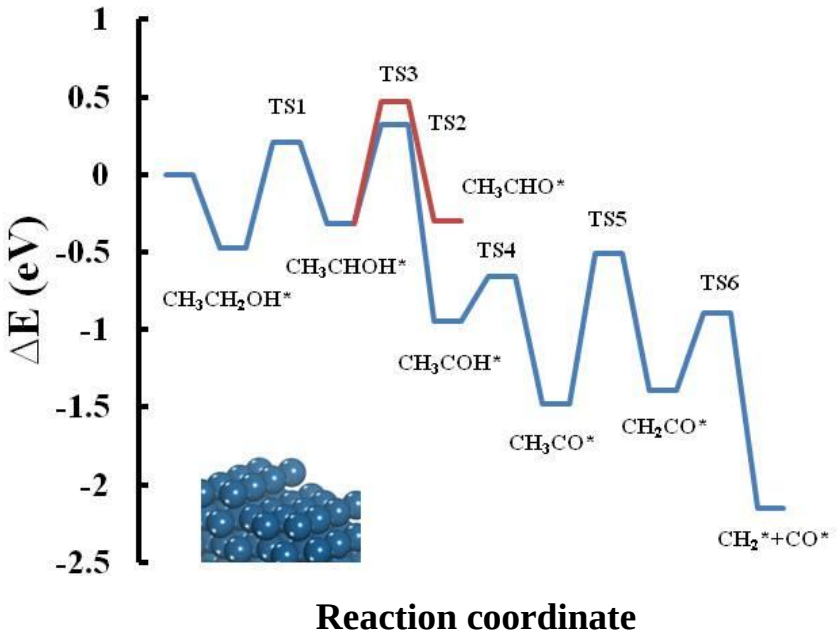

Figure S5. Energy profiles of ethanol adsorption and electrooxidation on Pt(211). Red line indicates the formation of acetaldehyde and the blue line indicates the formation of CO. Insert corresponds to the initial surface structure.

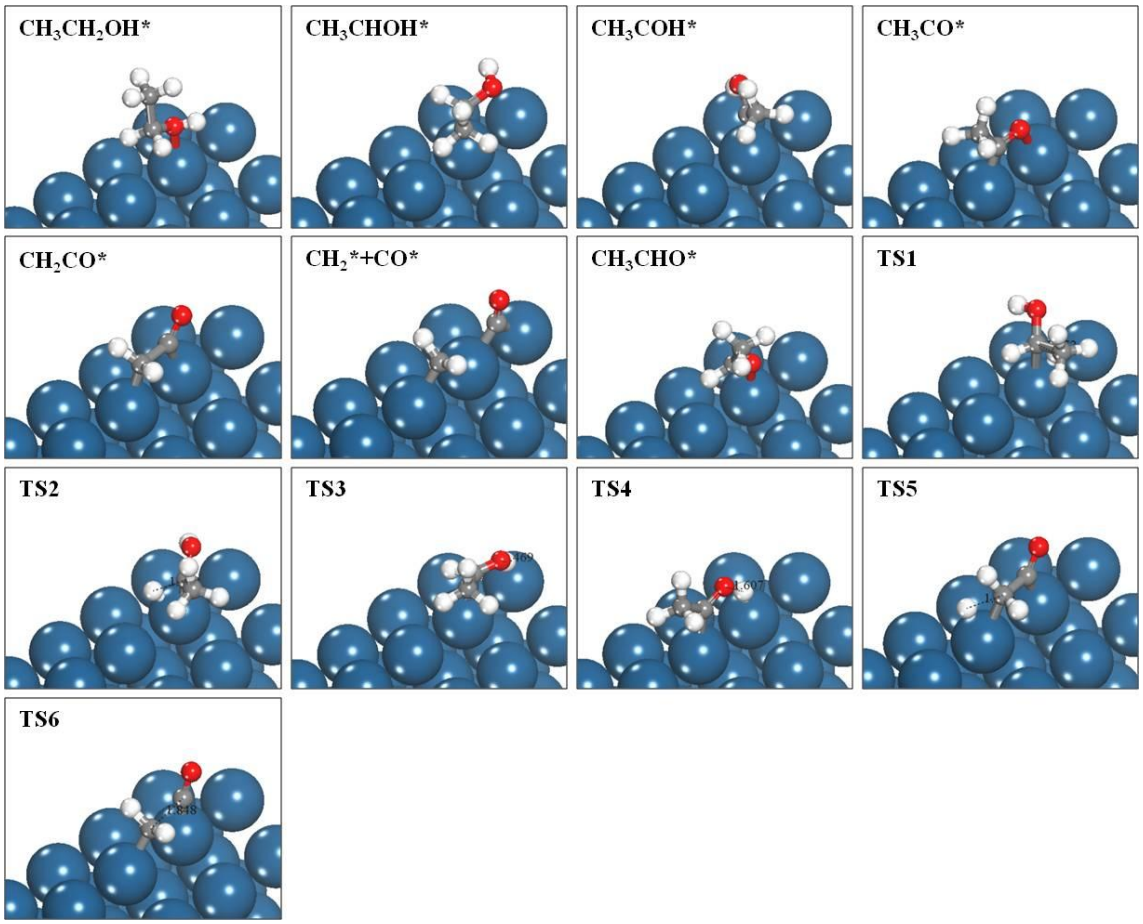

Figure S6. Optimized structures and located transition states during the ethanol adsorption and electrooxidation on Pt(211). The transition states, denoted as TS, correspond to the points in the reaction profile shown in Figure S5.