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

Supporting Information

Methanol oxidation on the Pt(321) surface: a theoretical approach on the role of surface morphology and surface coverage effects

Gabriele Tomaschun[a] and Thorsten Klüner[a,*]

[a] *Department of Chemistry, Carl von Ossietzky University Oldenburg, 26129 Oldenburg, Germany*

S1: CO adsorption geometries and adsorption energies on PtPd(321) and PtAu(321) surfaces

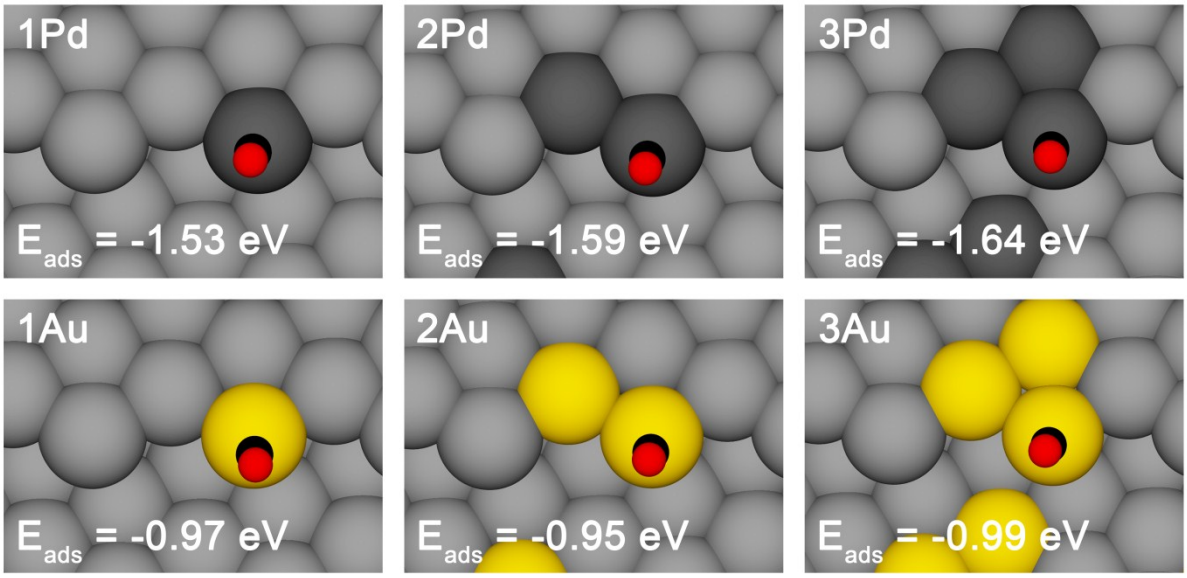

Figure S1: Geometries and adsorption energies of CO adsorbed on different PtPd(321) and PtAu(321) surfaces with 1, 2 and 3 Pt surface atoms replaced by Pd- and Au-atoms, respectively.

* Corresponding authors E-mail address: thorsten.kluener@uni-oldenburg.de

S2: Geometries of CO oxidation reactions on PtPd(321) and PtAu(321) surfaces

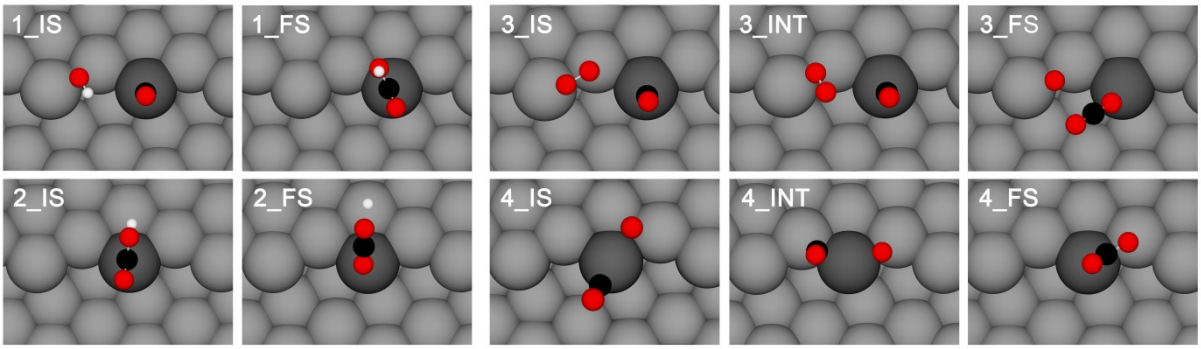

Figure S2: Initial (IS), intermediate (INT) and final (FS) states of CO oxidation with OH, O_2 and O on PtPd(321)-1Pd surface. The corresponding activation barriers can be found in Table 3.

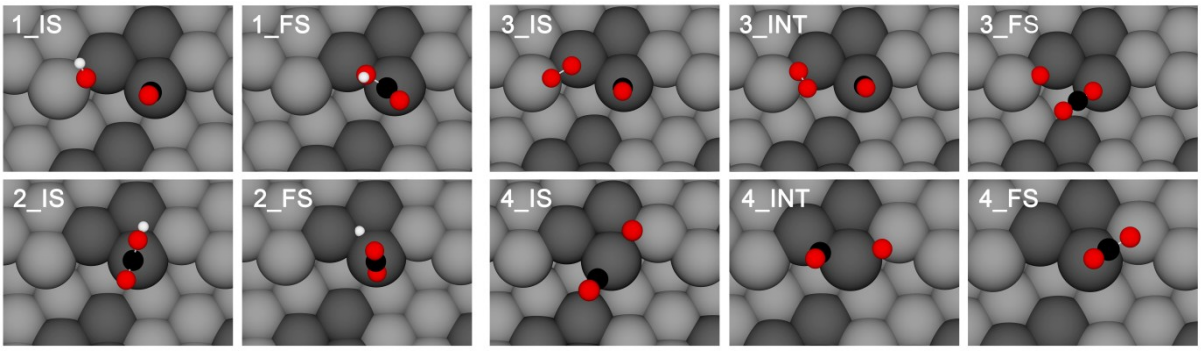

Figure S3: Initial (IS), intermediate (INT) and final (FS) states of CO oxidation with OH, O_2 and O on PtPd(321)-3Pd surface. The corresponding activation barriers can be found in Table 3.

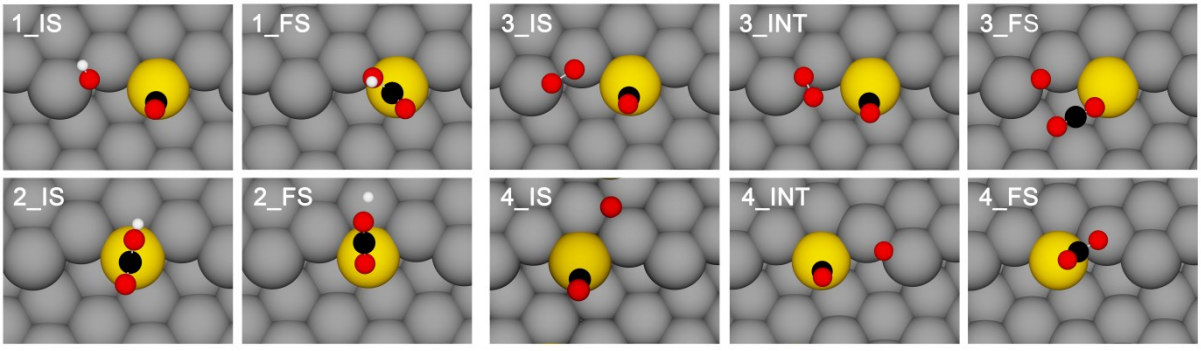

Figure S4: Initial (IS), intermediate (INT) and final (FS) states of CO oxidation with OH, O_2 and O on PtAu(321)-1Au surface. The corresponding activation barriers can be found in Table 3.

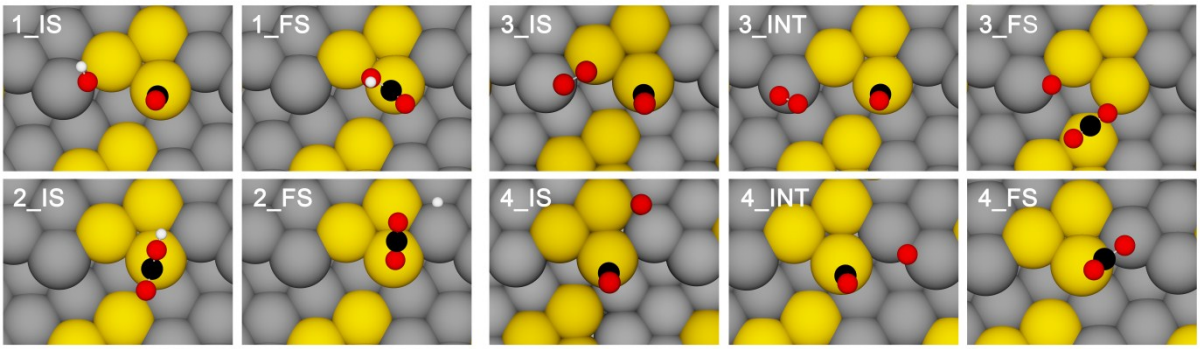

Figure S5: Initial (IS), intermediate (INT) and final (FS) states of CO oxidation with OH, O_2 and O on PtAu(321)-3Au surface. The corresponding activation barriers can be found in Table 3.

S3: CO-path vs. non-CO path

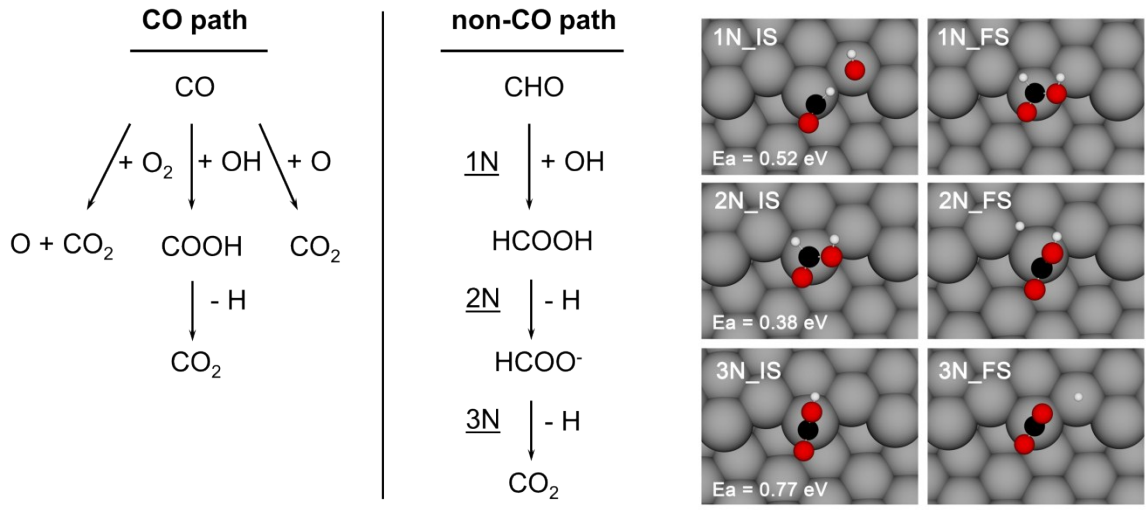

Figure S6: Left: Scheme of CO oxidation to CO_2 within the CO path. Right: Scheme and corresponding geometries of CO_2 generation within the non-CO pathway on Pt(321) surface. The respective activation energies (E_a) are depicted for all three reaction steps (1N-3N).

S4: OH coverage effect on RDS step (3N) of non-CO path

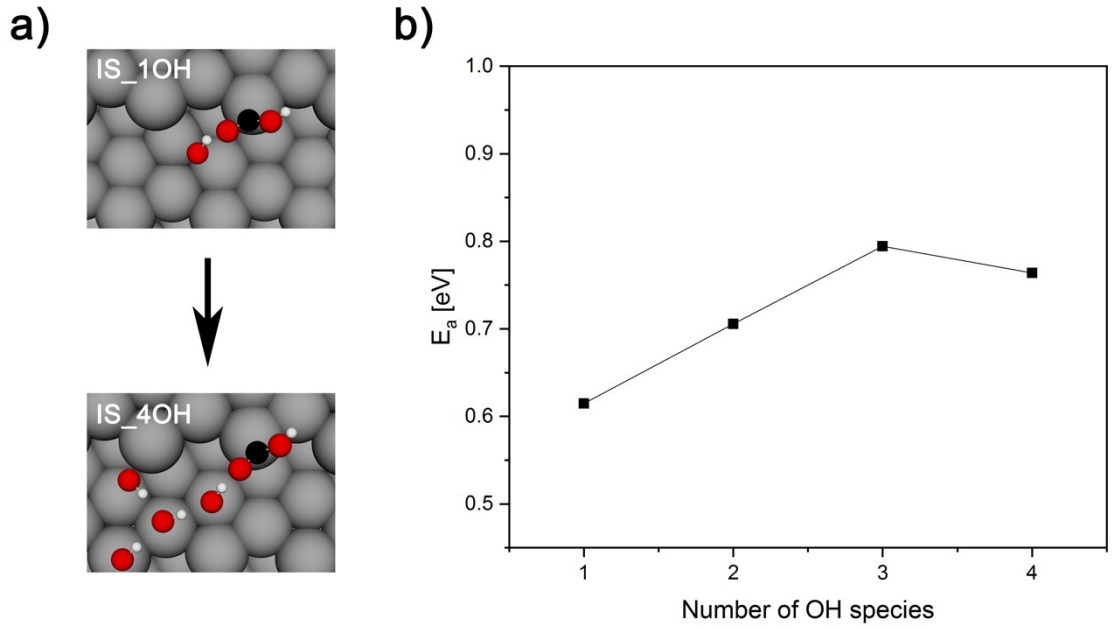

Figure S7: a) Geometries of the initial state (IS) of 3N reaction step with one (top) and four (bottom) OH molecules coadsorbed on the Pt(321) surface, respectively. b) Activation energies (E_a) of 3N reaction step (non-CO path) at different coverage of OH species coadsorbed on the Pt(321) surface.