Supplemental Material to
CO Oxidation Catalysed by Pd-based Bimetallic Nanoalloys

Dennis Palagin* and Jonathan P. K. Doye

I. Structures and relative energies of the $Pd_{5-x}Au_x$ and $Pd_{6-x}Au_x$ clusters adsorbed on the TiO_2 (110) surface

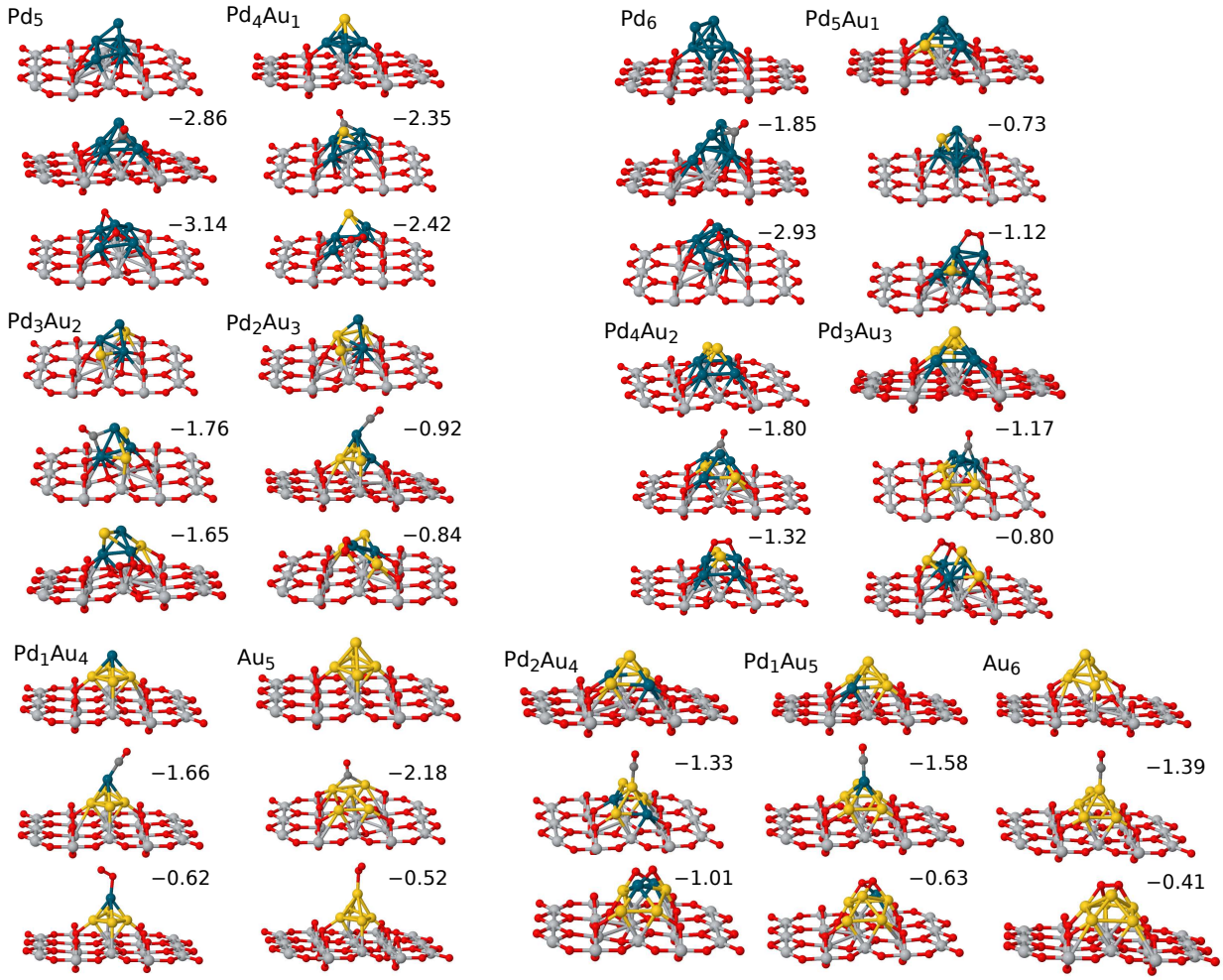

FIG. S1. Lowest-energy $Pd_{5-x}Au_x$ and $Pd_{6-x}Au_x$ clusters adsorbed on the TiO_2 (110) surface, and their aggregates with CO and O_2. Numbers indicate adsorption energies in eV.

* dennis.palagin@chem.ox.ac.uk

All calculations of adsorbed clusters were performed using the CASTEP package as specified in the Computational details section of the manuscript. Periodic slab models were applied for simulations of the TiO_2 (110) surface. Three stoichiometric bulk layers were used, with the top layer allowed to relax. As an initial configuration, the ground-state configuration of an individual cluster was placed 2 Å above the surface. For elimination of spurious interaction between slabs, the vacuum distance was set to 18 Å. All structures were optimized in the Γ-point approximation.

II. Pd_4Pt_2 intermediate aggregates reconfiguration

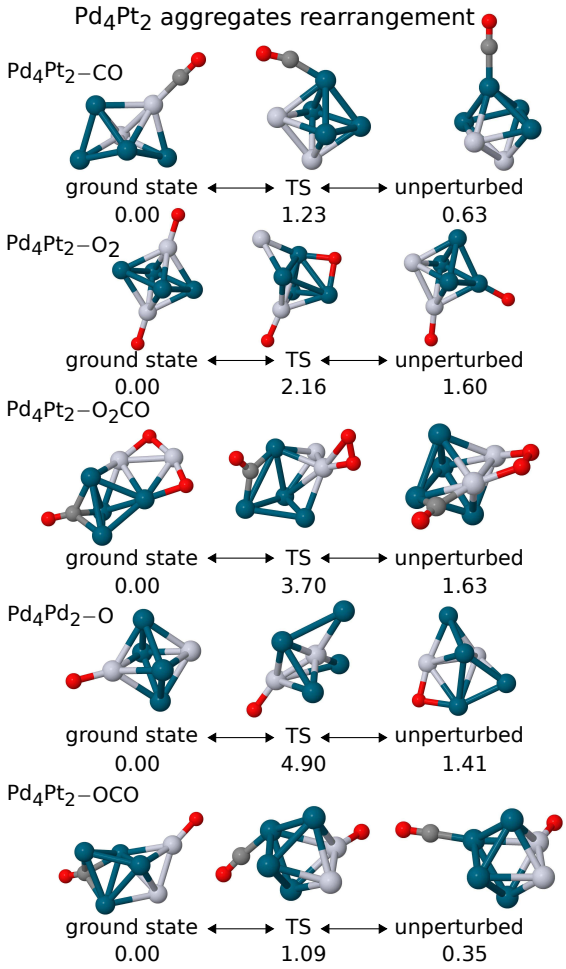

FIG. S2. Pd_4Pt_2 intermediate aggregates reconfiguration barriers.