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Oxidation of magnesia-supported Pd-clusters leads to the ultimate limit of epitaxy with a catalytic function

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Oxide-supported transition metal clusters and nanoparticles have recently attracted significant attention due to their important role as components of model-catalysts, sensors, solar-cells and magnetic recording devices. For small clusters, functionality and structure are closely interrelated. However, knowledge of the structure of the bare cluster is insufficient since the interaction with the chemical environment might cause drastic structural changes. Here we show by ab initio simulations based on the density functional theory that the reaction with molecular oxygen transforms small, non-crystalline, magnesia-supported Pd-clusters to crystalline Pd_xO_y nano-oxide clusters that are in epitaxy with the underlying support [1]. Restructuring of the Pd backbone is controlled by the electrostatic interaction with magnesia leading to a strong reduction of the O_2dissociation barrier. The supported Pd_xO_y clusters are likely to serve as Mars-van-Krevelen oxygen reservoirs in catalytic oxidation reactions as observed previously for PdO overlayers and demonstrated here for the oxidation of CO molecules. [1] B.Huber, P.Koskinen, H.Häkkinen, M.Moseler, Nature Materials, advanced online publication 4. Dec. 2005