DFT study on the Oxidative Removal of Pollutants

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CO, methane and ammonia oxidation over Pt-, Pd-, Rh- and Ru- based catalytic systems is experiencing renewed interest and growth. [1–3] This DFT study of mentioned surface oxidation processes uses Pt-, Pd-, Rh- and Ru- surfaces as well as supported single-atoms [4-5] and clusters [6] as model catalysts. Furthermore, the investigations are often accompanied by an in-depth analysis using microkinetic models. Several suggestions have been reported for the active site of noble-metal-based systems for NH_3 oxidation**.** The unequivocal identification of active sites responsible for the high catalytic activity of Pt-based systems is furthermore complicated by the fact that these systems are changing with reaction conditions, as e.g., shown recently for the case of Pt/CeO_2.[7] Consequently, several model systems need to be employed to investigate the reaction mechanism on mentioned catalysts. The simplest models will be extended metal surfaces of various terminations (e.g. (111), (100), (211)) and supported single atoms such as Pt/CeO_2.[8] Oxide supported clusters also need to be addressed as the quantum-size effects for particles smaller than 1.6 nm (or approx. 150 Pt atoms) are revealed to affect the binding energies of reactants significantly. [9-10]

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