## Abstract Submitted for the MAR06 Meeting of The American Physical Society

One-dimensional  $PtO_2$  oxide at Pt steps: formation and reaction with CO J.G. WANG, W.X. LI, T.M. PEDERSEN, B. HAMMER, University of Aarhus, Denmark, J. KLIKOVITS, M. SCHMID, Technische Universität Wien, Austria, M. BORG, J. GUSTAFSON, A. MIKKELSEN, J. WEISSENRIEDER, E. LUNDGREN, J.N. ANDERSEN, Lund University, Sweden — The structure and catalytic activity of a one-dimensional  $PtO_2$  oxide, which forms along the steps on the Pt(332) surface, is studied using HRCLS and DFT [1]. Our investigations reveal a much higher CO-oxidation activity of the one-dimensional oxide as compared to the chemisorbed oxygen phase of Pt(111). The reason could be explained by DFT by the detection of a significantly lower barrier for the  $CO_2$  formation using O from the oxide stripe, as compared to the O chemisorbed on the terrace. Finally, the one-dimensional oxide is predicted to be stable at conditions between chemisorbed oxygen and the bulk oxide, which at 500 K includes ambient oxygen pressures. This range is expected to be similar on other step structures of Pt. Hence the one-dimensional oxide could be of major importance for the catalytic activity of Pt nano particles, as used in industrial catalytic devices. [1] J. G. Wang et al., Phys. Rev. Lett. In Press. This work was financially supported by the Swedish Research Council, the Danish Research Council, Dansk Center for Scientific Computing, the EC contract No. NMP3-CT-2003-505670 (NANO2), and the Austrian Fonds zur Förorderung der Wissenschaftlichen Forschung.

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