

## **Review of Doctoral thesis by Tomas Duchon**

**Title: Electronic and structural properties of model catalysts based on cerium oxide**

**Univeristy: Charles University, Prague**

**Supervisor: Katerina Veltruska**

The thesis deals with furthering our understanding heterogeneous catalysis. A process that had a pivotal role on the wealth of our modern society. Despite the ubiquitous use of heterogenous catalysis the mechanisms governing its success are often not well understood. Tomas Duchons thesis tries to, and successfully closes this gap somewhat - a great achievement. The work is interesting both from a scientific and technical point of view and is very timely. The work has been carried out in a systematic way and the thesis is well written. The author show maturity and the text reflects a deep knowledge subject and of the experimental techniques used to carry out the core of the measurements but also demonstrate a considerable understanding of the literature on computer simulations (note that this is the expert area of the reviewer) which adds to the reading experience and to the understanding of the results.

The graphical presentation is generally of high quality (except for Figure 1.1, see separate comment below).

The aim are clearly stated and the structure of the thesis is clear. The quality and sheer amount of publications (16 of them) is well beyond what is customary in the Swedish system, which I am most aquatinted with. There is now doubt on my part that the thesis must clearly fulfil the requirements on scientific quality in any system.

The thesis focus on an important class of catalytic converters based on cerium oxide (ceria). Using novel techniques to prepare film of controlled amount of oxygen vacancies (a key defect in cerium oxide) new insight have been provided. Most notable a careful assessment of the transition, on an atomic scale, in the transition from a fully oxidized ceria film to a fully reduced one.

## Questions and comments:

1. In figure 1.1 and in the main text on page 4 in the description of the Mars van Krevelen mechanism and CO oxidation the connection to catalysis is somewhat forgotten since there is no mention of the crucial reoxidation process which is needed to close the catalytic cycle. In my opinion, the text and figure would have benefited from addressing this aspect.
2. In the introduction there are many claims regarding the importance of catalysis. However, there are no references supporting these claims. Again, the text would have benefited from including some more references.

As a whole, the work is very solid and in my opinion Tomas Duchon have fulfilled all the necessary requirements for granting a PhD. degree according to the applicable laws. I would therefore recommend that the work should be accepted for the defense.

Uppsala (Sweden) 09.08.2017

Jolla Kullgren PhD.