



Contribution ID: 145

Type: **not specified**

## **Theoretical Investigation of the Reducibility of PtOx single atom catalysts supported on Ceria (111), (110) and (100)**

*Monday, November 28, 2022 1:30 PM (30 minutes)*

Internal combustion engines use highly dispersed noble metals such as Pt, Pd and Rh as catalytic active substances and oxides such as ceria, titania and alumina as carriers for exhaust gas after-treatment. The identification of the active species is exacerbated by the fact that catalysts undergo a dynamic structural change under reaction conditions.

SACs are on the very boundary between heterogeneous and homogeneous catalysis. Thinking about complex chemistry, the support poses a multidentate ligand which interactively takes part into the reaction and enhance the activity of the catalyst. Ceria and Pt are known as very active catalysts. But the exact nature is yet unknown and needs plenty small steps from different fields to be enlightened. Here we start at the very bottom and provide a thorough foundation, which will then lead the direction of further investigations, meaning other noble metals, other supports, or other simulation methods as kinetics or input for characterization methods or testing of the activity.

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**Session Classification:** Poster session