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Type: **Poster Presentation**

## Computational modelling for understanding the fundamentals of methane oxidation over palladium oxide

*Tuesday, 4 July 2017 17:10 (1h 50m)*

One of the main challenges in natural gas engine after treatment is the combustion of methane at lower temperatures. The presence of water and sulphur in the engine exhaust lowers the catalyst performances. With various computational simulations, we are developing models that will assist in understanding the fundamentals of these reactions and making predictions for further improvements of the catalysts.

The grid-based projector-augmented wave (GPAW) method has been used to determine the reaction path of methane oxidation over PdO surfaces. This lead to an understanding of the complete catalytic combustion of methane at a range of temperatures as well as the resultant production of CO<sub>2</sub> and H<sub>2</sub>O. A series of dopants has been introduced to the surface model to determine the effect of doping on PdO. Reaction profiles are mapped out and preliminary results will be presented.

**Apply to be considered for a student award (Yes / No)?**

No

**Level for award (Hons, MSc, PhD, N/A)?**

N/A

**Would you like to submit a short paper for the Conference Proceedings (Yes / No)?**

No

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**Session Classification:** Poster Session 1

**Track Classification:** Track A - Division for Physics of Condensed Matter and Materials