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Multiscale Simulation of Functional Coatings For Catalytic Applications

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Catalytic coated monoliths represent an important class of materials for clean chemical production and emission control. The computational description, simulation and prediction of behaviour relies on phenomena occurring over a number of time and length scales:

1) At the electronic and molecular level the bond making and breaking at a catalyst surface, responsible for the function of the coating.
2) At the nano scale micro-kinetic modelling to capture the kinetics of the chemistry.
3) At the micro scale transport of gases through the porous catalytic coating.
4) At the reactor scale transport through the monolith channels.

Combining computational methods from the field of materials science and chemistry at the lower end of scale, with chemical engineering models of porous media and diffusion at the micro scale, we can construct and parameterise Computational Fluid Dynamics models that allow the interplay of the different scales to be captured.

In this presentation results will be present from work conducted in-house where we have used models at the atomic-scale to help inform development of novel catalysts for combustion of natural gas in vehicles. Through the EU funded programmes Marketplace [1] and ReaxPro [2] we are making steps towards interoperable linkers between scales. Results will be presented from each of the scales and how we are now starting to link together these simulations to obtain a holistic view of the catalyst function and performance.

REFERENCES

[1] https://www.the-marketplace-project.eu/.
[2] https://www.reaxpro.eu/.