

Modelling of CO₂ conversion to Methanol

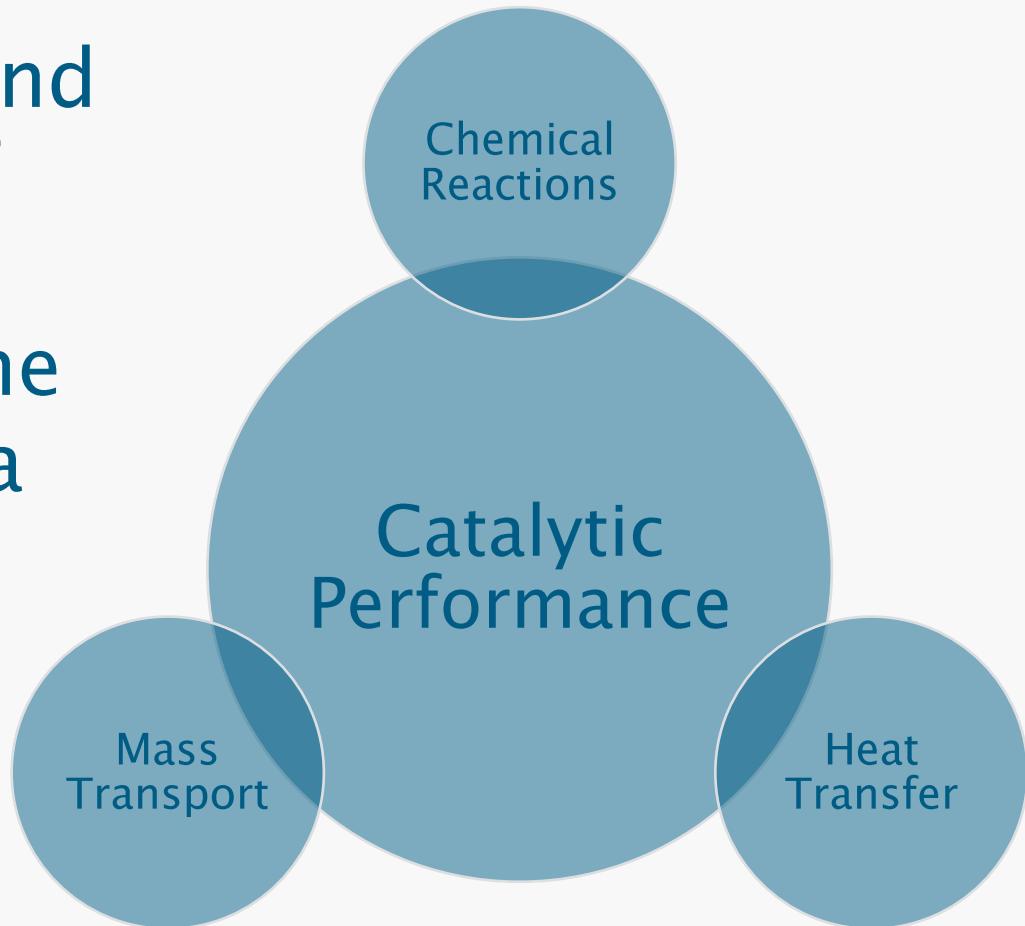
Chris Pamouktsis

Faculty of Engineering

L.M. Armstrong, R. Raja, E.S Richardson

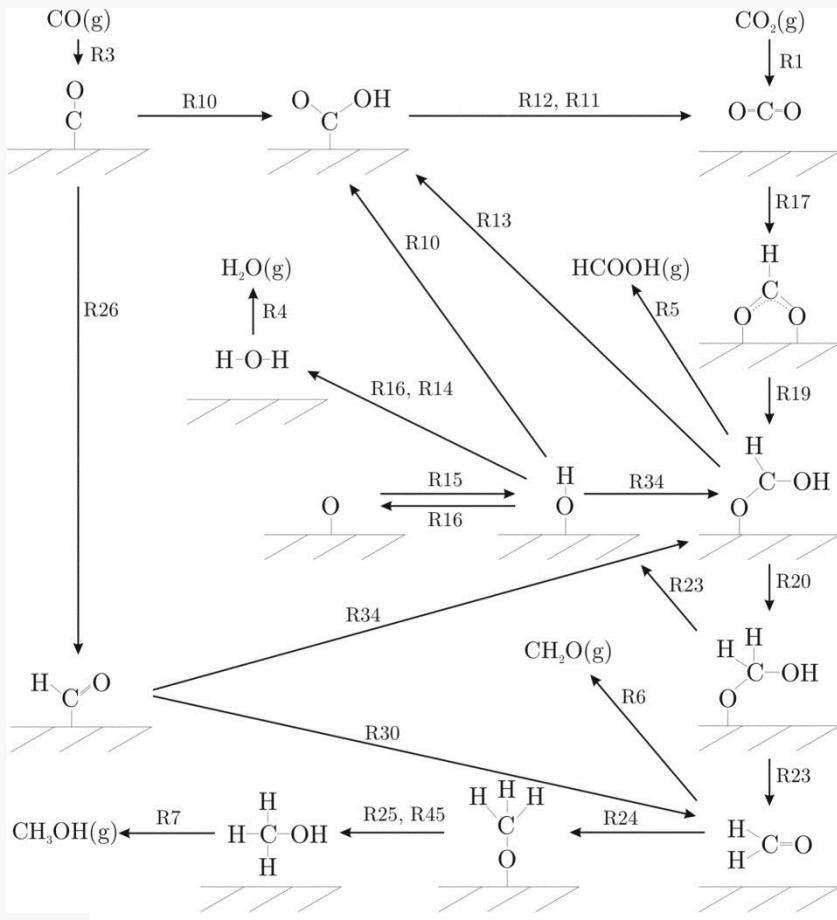
Aim

- Understanding and quantification of interrelated phenomena in the performance of a catalytic system



Method – Modelling

- A different extensive network of fast elementary reactions to be adequately accounted for described
- DFT approach has
- Much more fully described the elementary chemical model used for this work



Method – Synthetic

- Synthesis of ordered mesoporous materials to be used as catalysts

