Spectroscopic and theoretical characterization of heterogeneous catalysts based on supported metals

PhD in Sustainable Chemistry

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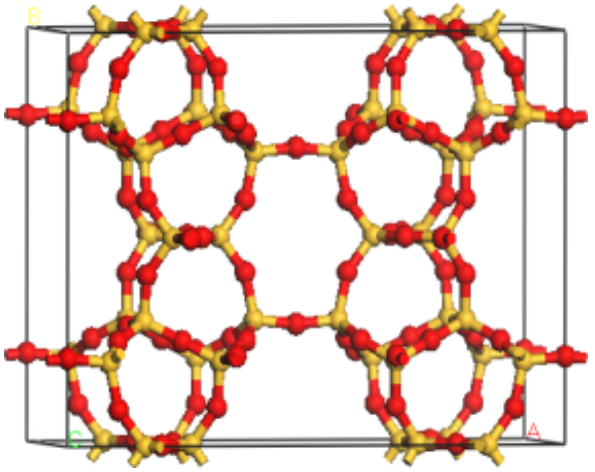

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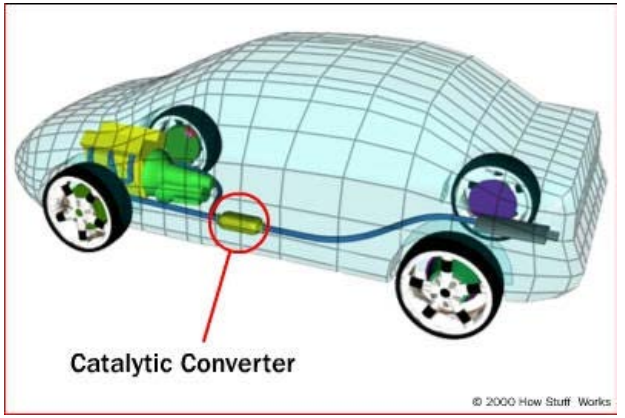
Motivation

What 's wrong ?

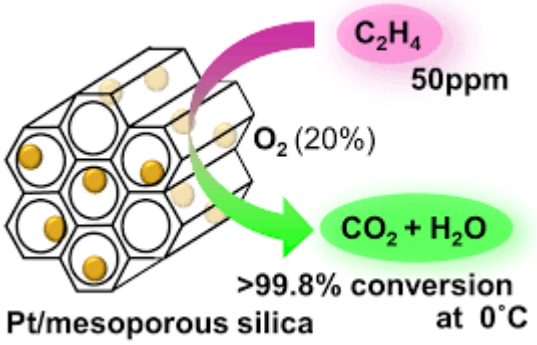
Solution



Catalysts

Biomass waste

Solution
again



Catalysis

Objective

To study the chemical properties of **solid materials (heterogeneous catalysts)** made up by metal species on inorganic support by means of **spectroscopic** and **computational techniques.**

But why heterogeneous catalysis ????

Heterogenenous catalysis	**vs**	**Homogeneous Catalysis**
Easy to reuse and/or recycle		Difficult and expensive
Good thermal stability		Poor thermal stability
Multiple active site		Single active site
Cleaner		Complex separation of products
Nanoscale catalysts		

What to do?

Computational Modelling

Density Functional Theory

-Most favorable interactions

-Most stable species

-Energies

-Frequencies IR, Raman NMR, XPS, EPR

Spectroscopy

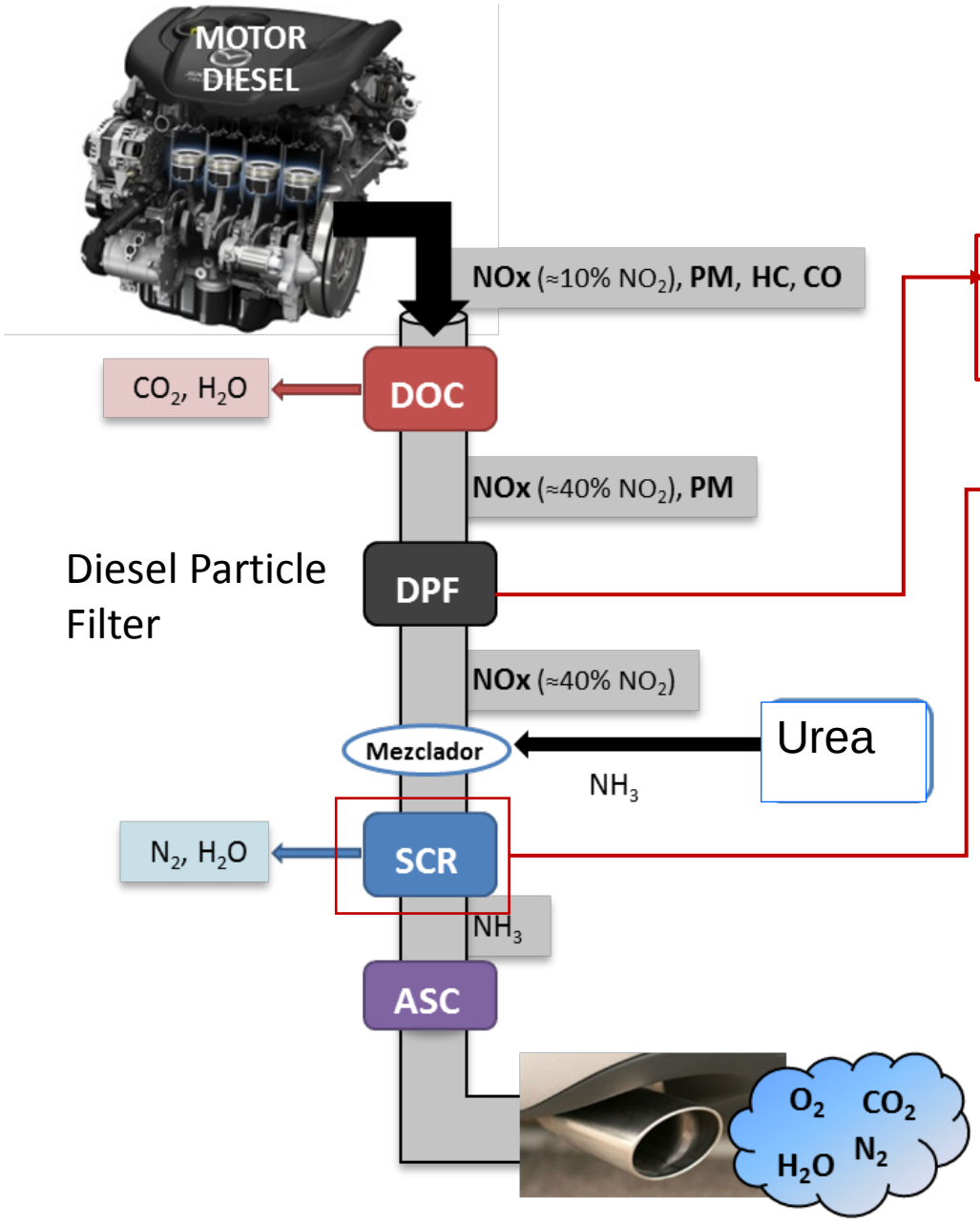
FTIR, RAMAN, UV-VIS, NMR, XPS, EPR, AUGER

Experimental Information about the structure of reactants and products

Reaction Mechanism
We will know how the reaction occurs

We will be able to modify the catalyst to make it more efficient

Pollution due to NOx



T≈ 700ºC. water is released

Carries Cu cation outside the structure of the catalyst

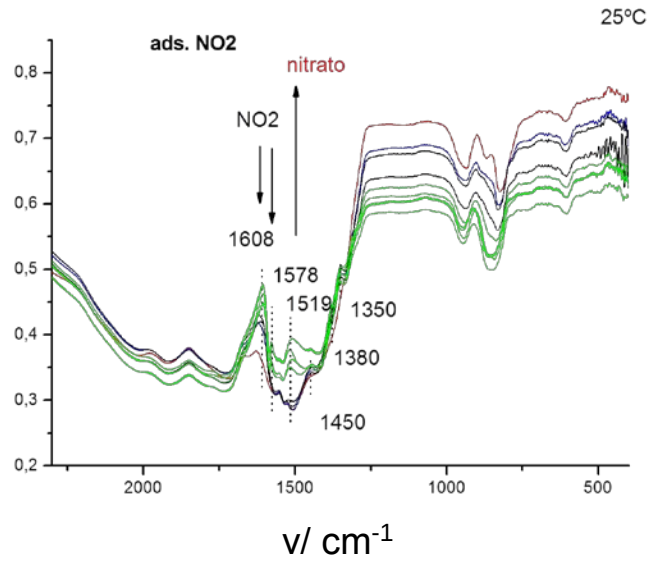
Solution: direct synthesis

Improve performance at low T when starting the car

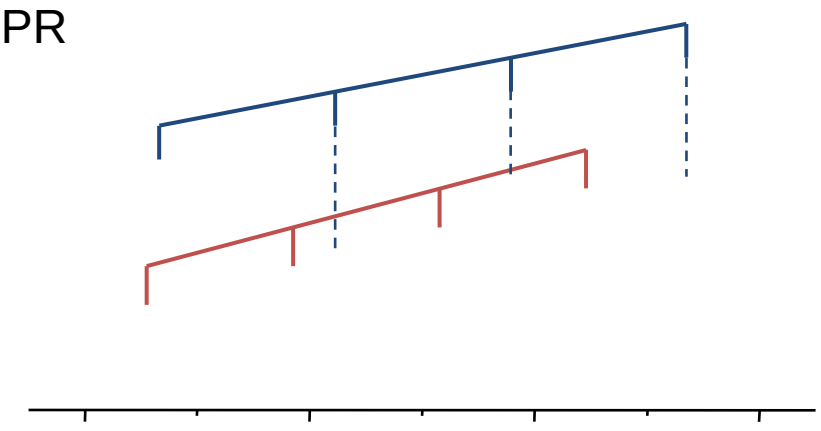
What do we already know?

Spectroscopic information

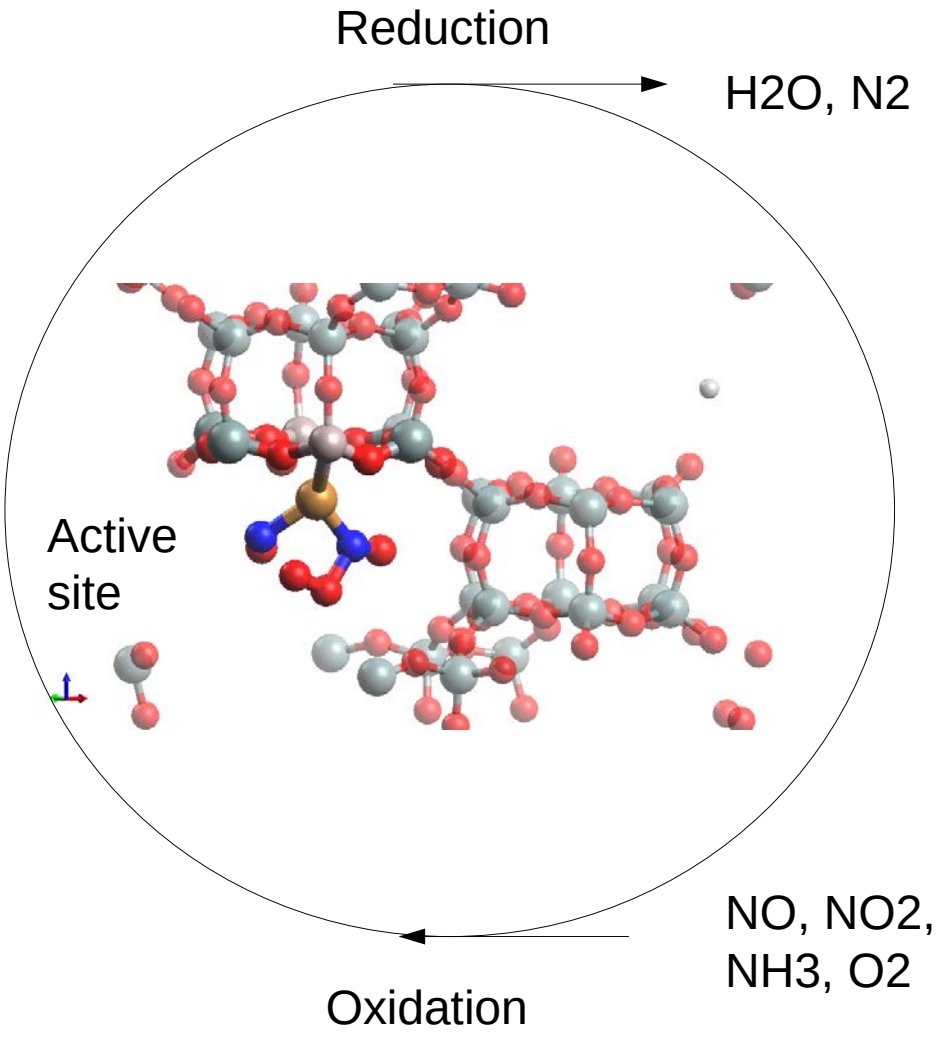
IR



EPR



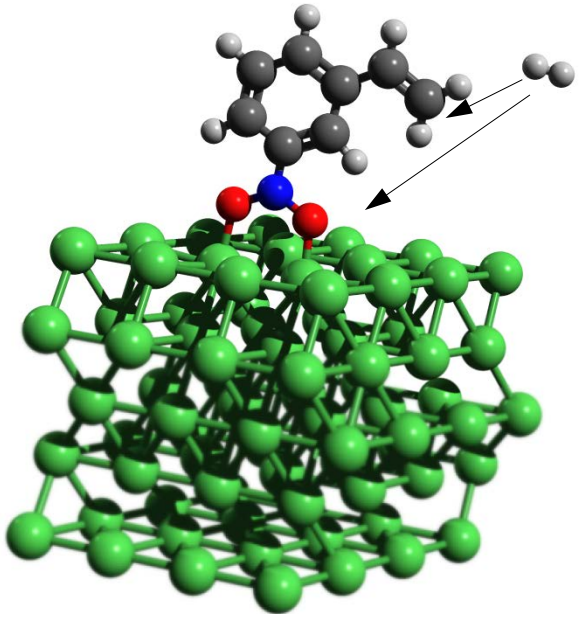
Selective Catalytic Reduction



What's next?

Study the complete catalytic cycleIdentify the active, selective and most efficient sites → Improve efficiency of the catalyst and reduce the emissions of nitrogen oxides by diesel vehicles if catalysts are used

Other systems:



Intermediate for →

Pharmaceuticals

Polymers

Fine chemicals

Thanks