

Practical course
Characterization of catalysts and surfaces course

Monday, 9.45-10.30 am + Case Study week (9.11 on)

	Date 1	Date 2	Date 3	Date 4	Date 5	
NMR	1	2	3	4	5	
XRD	2	3	1	5	4	
BET	3	1	2			

group 1 –

group 2 –

group 3 –

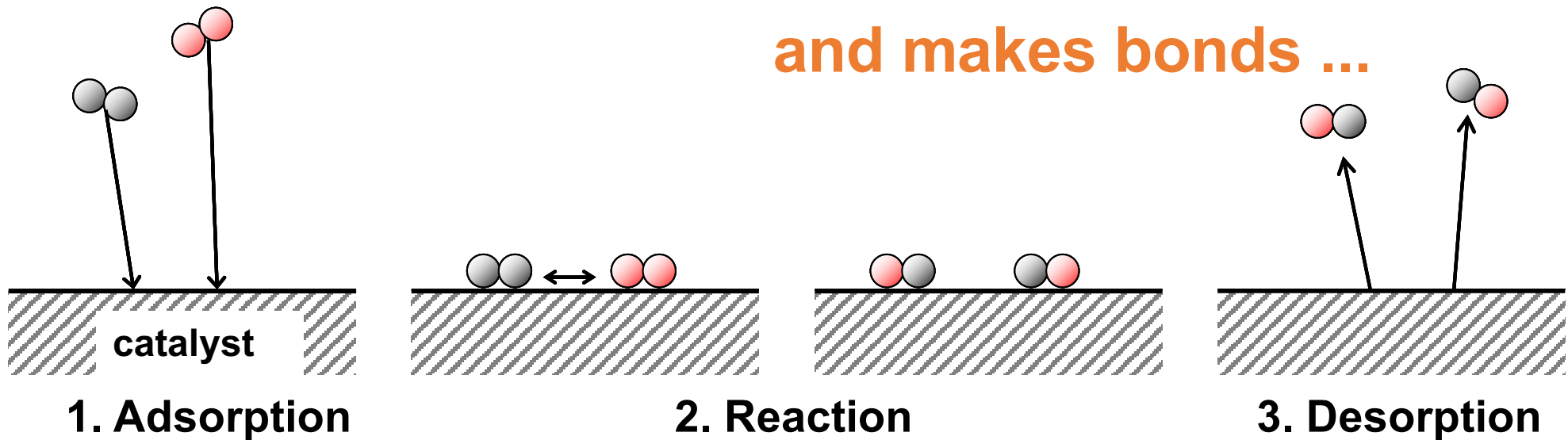
group 4 –

group 5 –

What does a catalyst do?

A catalyst breaks bonds ...

and makes bonds ...

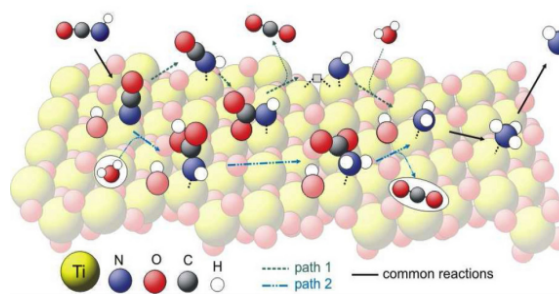
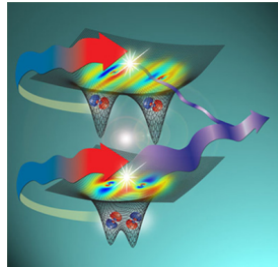
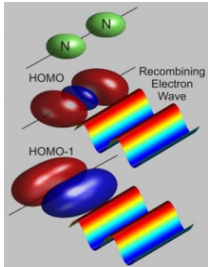


What is an active site ??

Knowledge of reaction mechanism essential to appreciate characterization

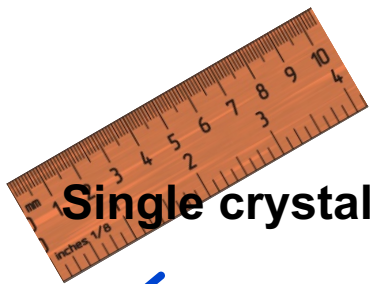
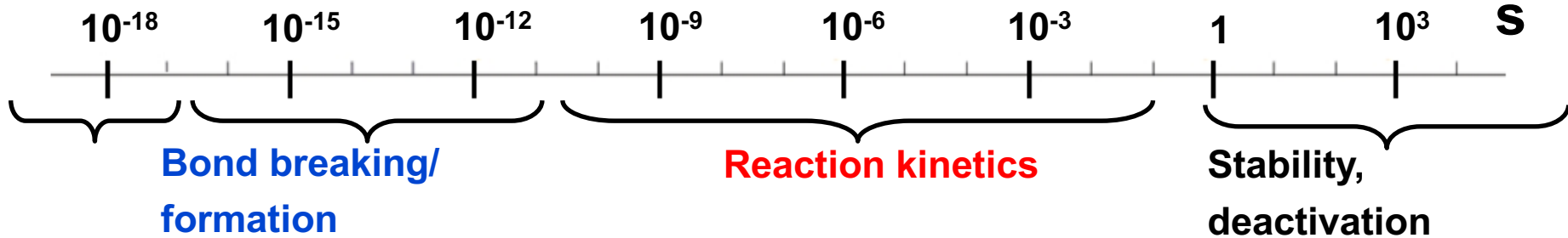


Catalysis: time and length scales

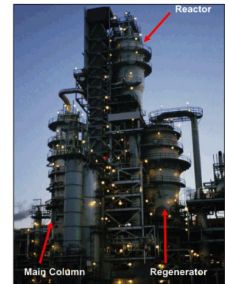
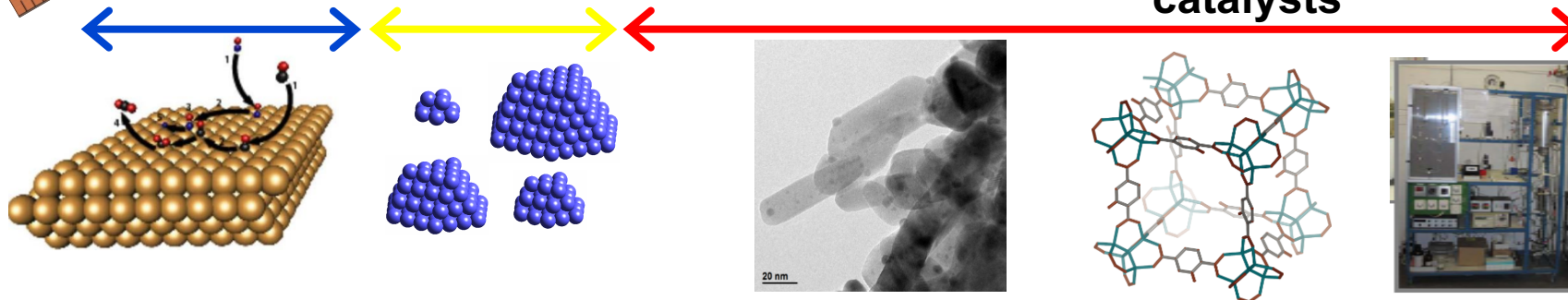


Fundamental

Applied

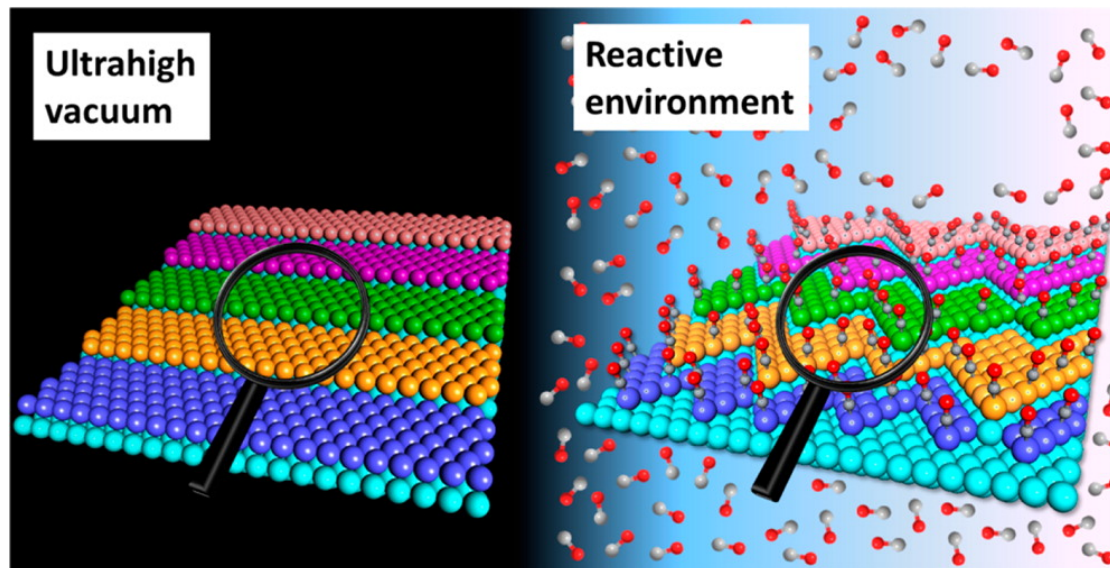


Single crystals ··· **clusters** ··· **supported metals** ··· **single site catalysts** ··· **reactors**



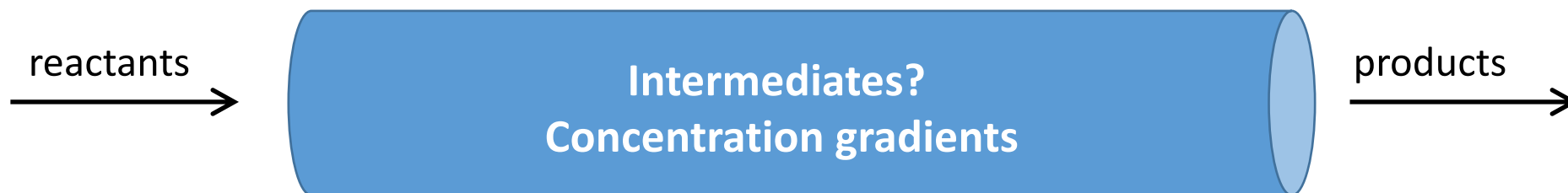
In situ spectroscopy

- Catalyst structure is a function of its environment
- Only structure measured under reaction conditions can give insight into activity
- Conversion changes the gas environment



Shiran Zhang; Luan Nguyen; Yuan Zhu; Sihui Zhan; Chia-Kuang (Frank) Tsung; Franklin (Feng) Tao; *Acc. Chem. Res.* **2013**, 46, 1731-1739.

What about a plug-flow reactor?



Catalyst structure is not necessarily the same everywhere in a reactor!!

Grundwaldt (2007) ; van Bokhoven (2010)

Catalyst characterization

- Structure of the catalyst *surface vs bulk*
- Structure of reaction intermediates

Points of care:

Spectator species *not everything one sees is active*

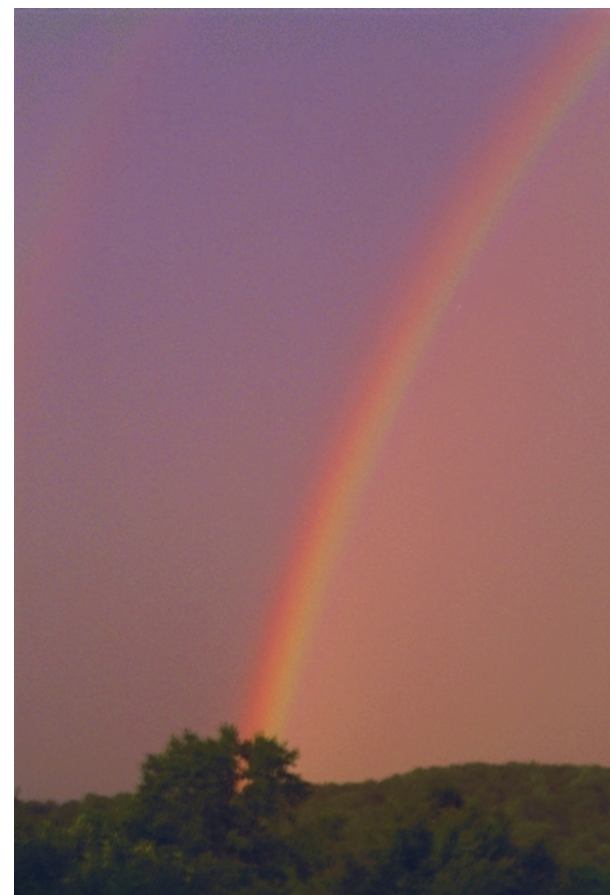
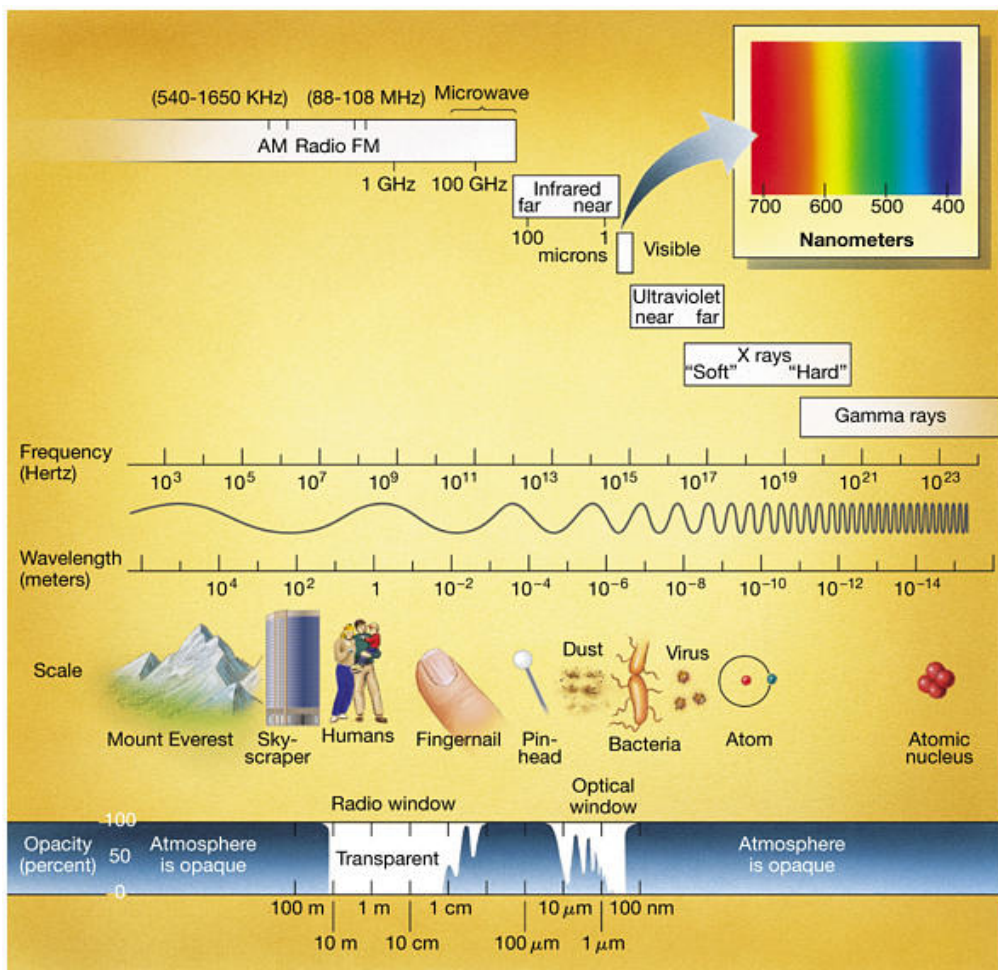
Short-lived species *the active intermediate may be short-lived*

In situ / operando *catalyst structure changes with conditions*

Shining light on catalysts

Catalyst characterization:

UVvis, infrared, XRD, TGA, TPD-MS, TPR/O, TEM, NMR, XPS, XAS, XES,



What is catalysis?

Why should they be characterized?

What characterization tools are needed?

Catalyst surface, bulk, adsorbates (intermediates)

The catalytic cycle: structure of the catalyst changes with gas environment

Catalytic cycle: (TON, TOF)