

# Practical course

## Characterization of catalysts and surfaces course

Monday, 09:45-10:30 am

	Assistent	Summary	25.9	2.10	9.10	16.10	23.10
NMR	Teng	Solid state NMR (Al and C) for assessing the synthesis of zeolite Room D130		1	2 + 4	3	
XRD	Amy	XRD and phase identification of zeolites E128	3	2	1		4
BET	Manoj	Surface area and porosity analysis of zeolites: Sample preparation and data analysis E122	2	4	3	1	
IR	Petr	Sample Prep and spectrum analysis E128	1	3		2 +4	

group 1 –

group 2 –

group 3 –

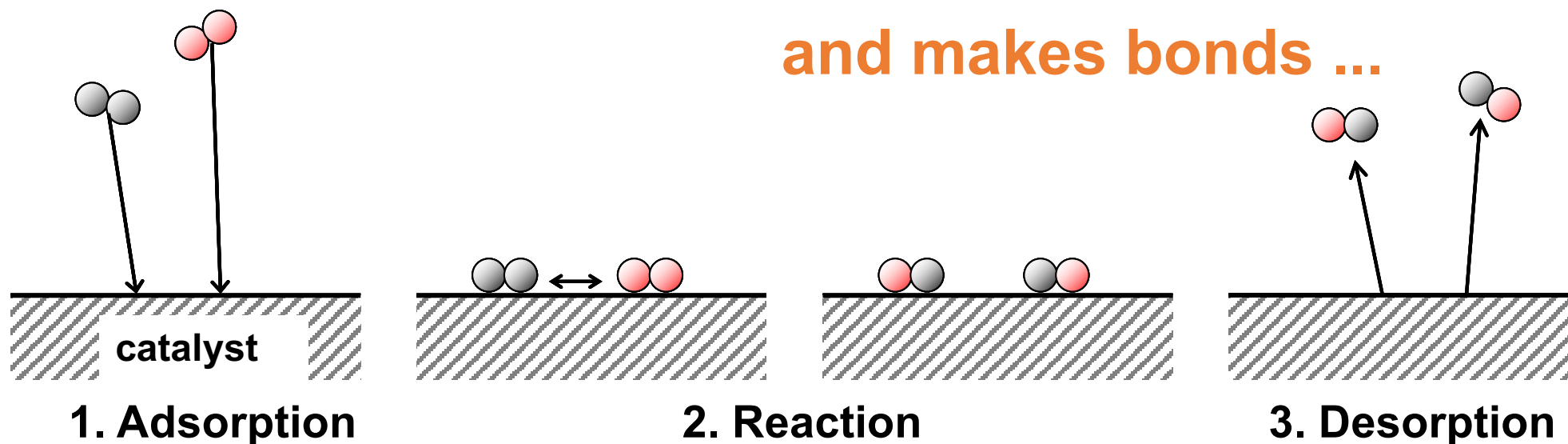
group 4 –

group 5 –

# What does a catalyst do?

A catalyst breaks bonds ...

and makes bonds ...



*What is an active site ??*

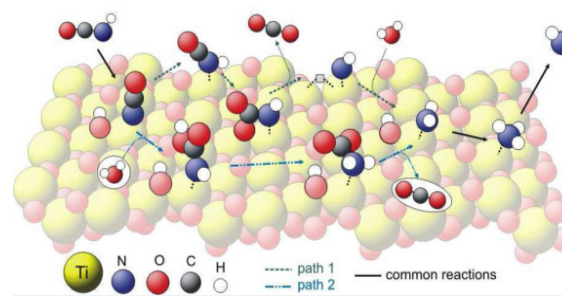
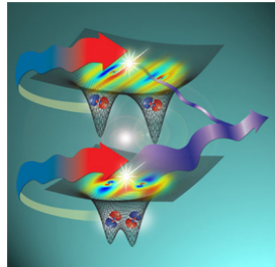
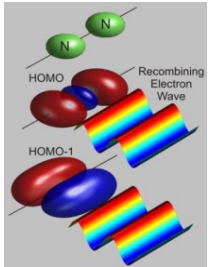
*Knowledge of reaction mechanism essential to appreciate characterization*

*TON: turnover number*

*TOF: turnover frequency*

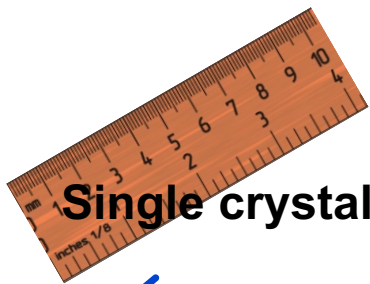
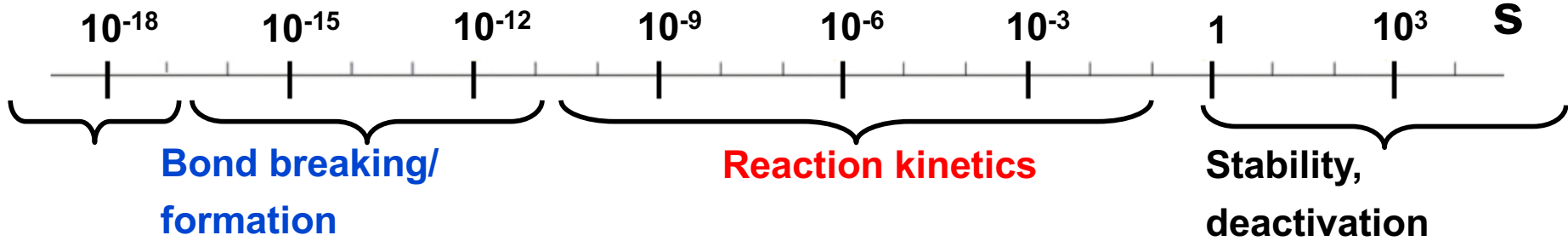


# Catalysis: time and length scales

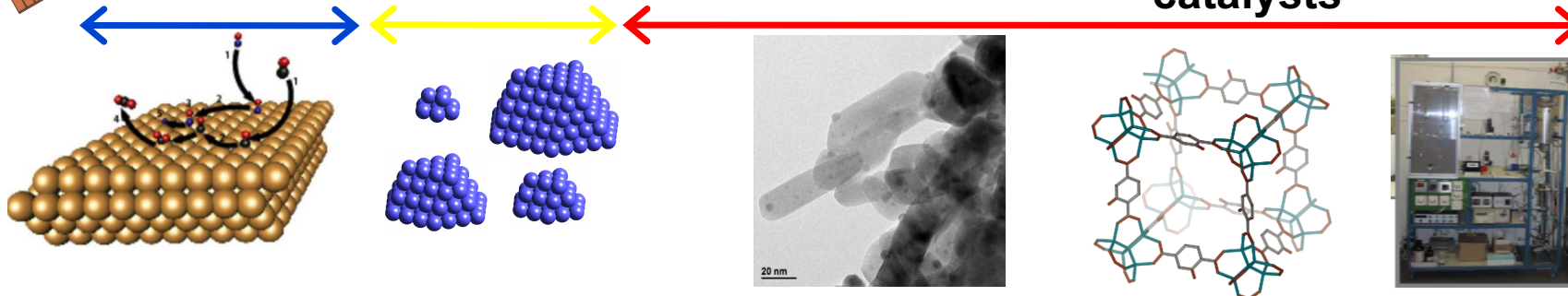


**Fundamental**

**Applied**

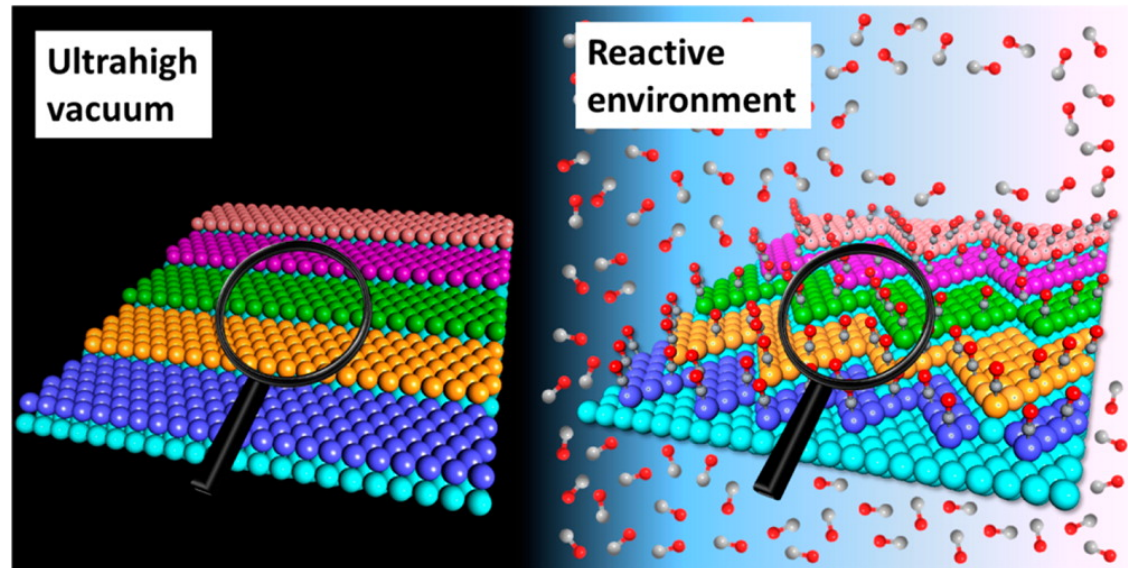


**Single crystals ··· clusters ··· supported metals ··· single site catalysts ··· reactors**



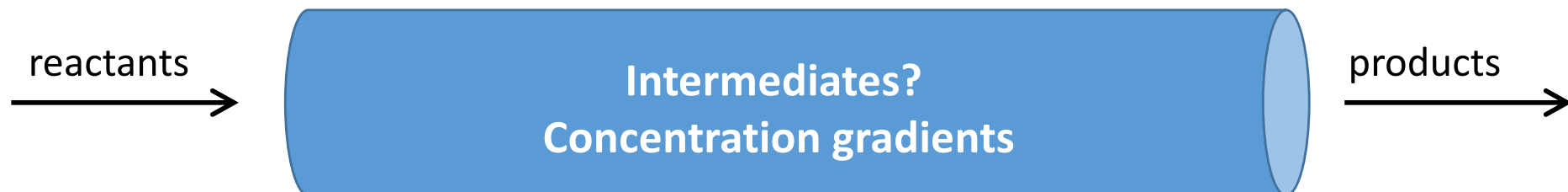
# In situ spectroscopy

- 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*

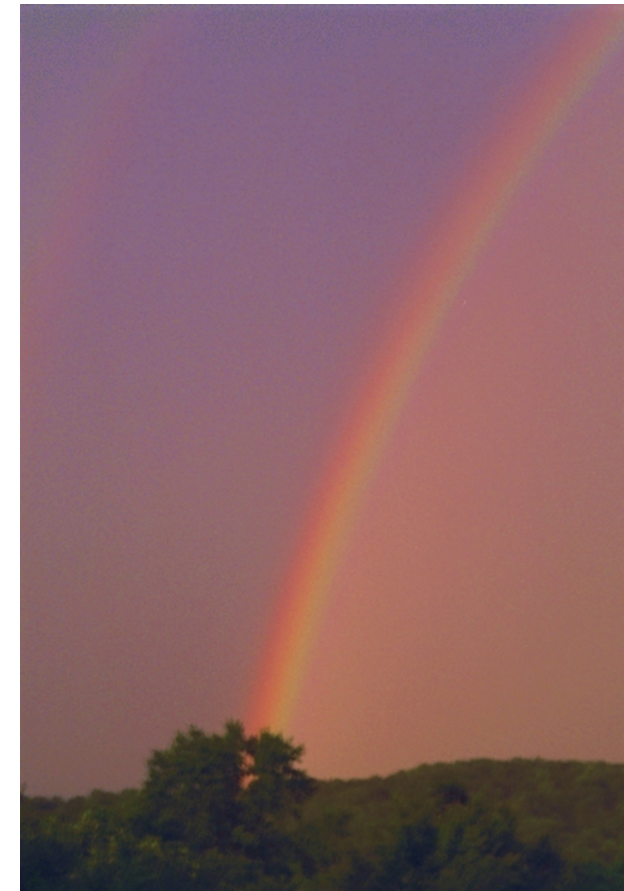
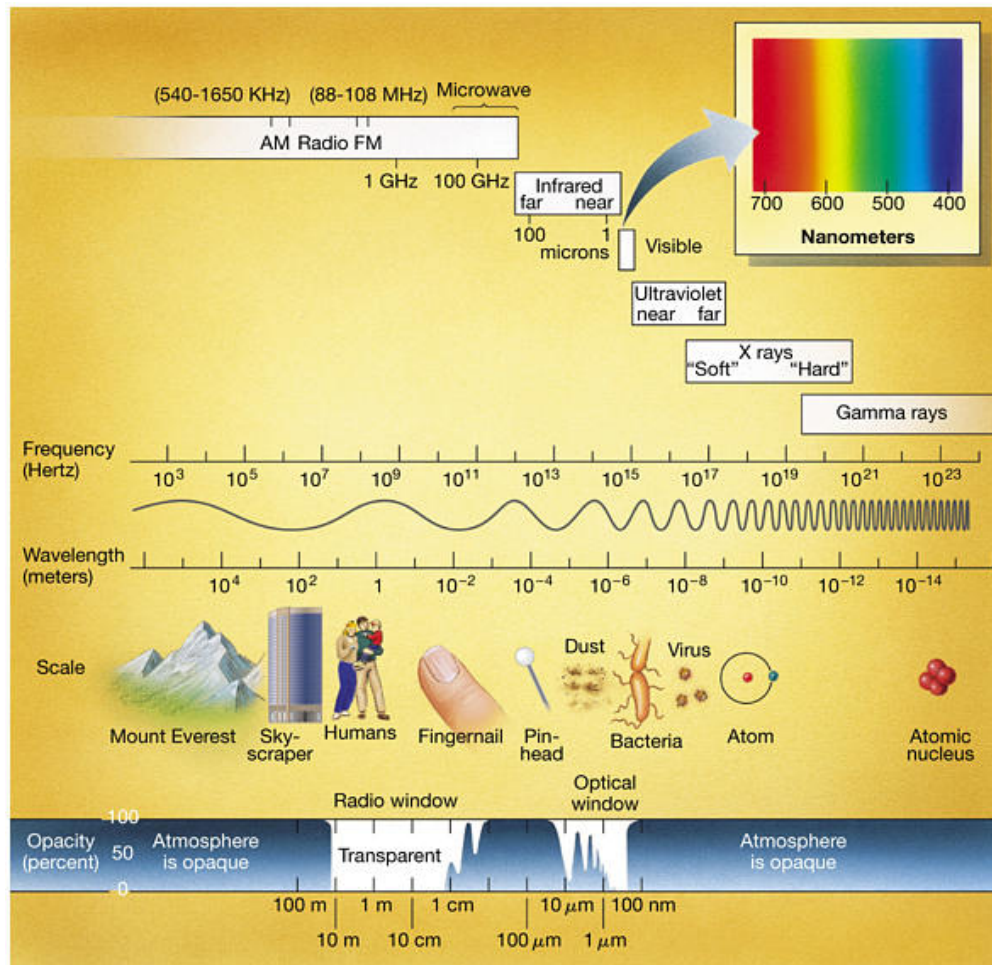
In situ / operando *catalyst structure changes with conditions*

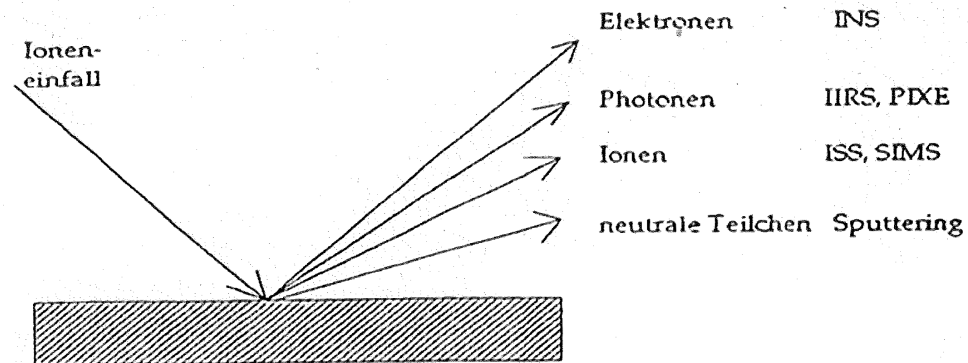
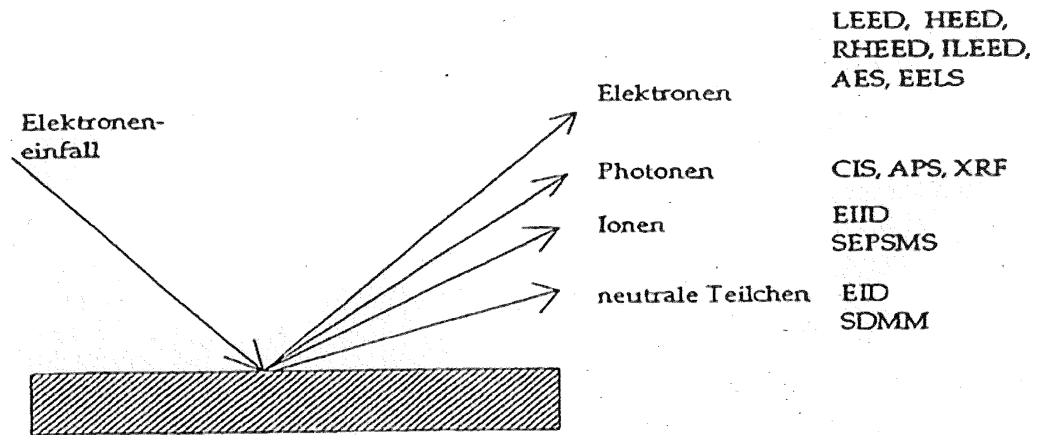
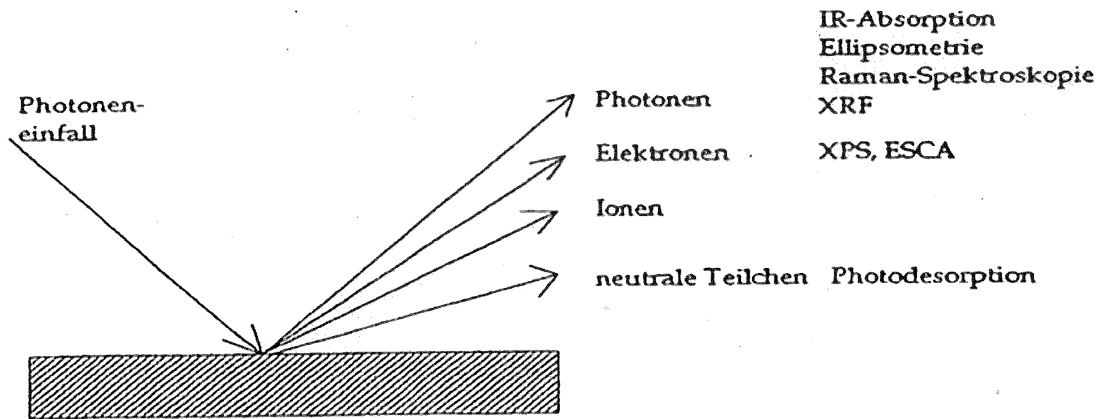


# Shining light on catalysts

## 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)