Freie Universität Berlin

# From 2D materials to Energy Storage

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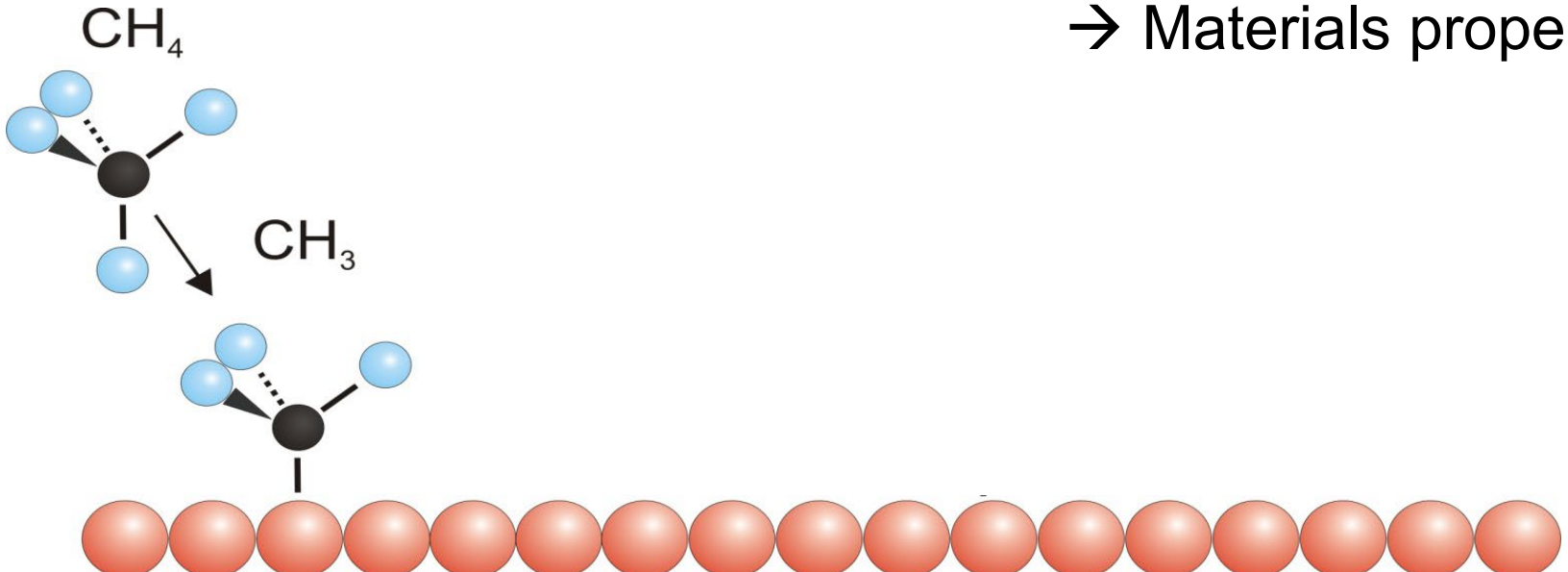
CLINT Catalysis at Liquid Interfaces

# Motivation

## Microscopic understanding

→ Adsorption / Dissociation
→ Chemical bonds
→ Reaction
→ Diffusion
→ Desorption




## Chemical Kinetics in Catalysis

→ Intermediates
→ Activation energy

## Growth / Functionalization

→ 2D materials

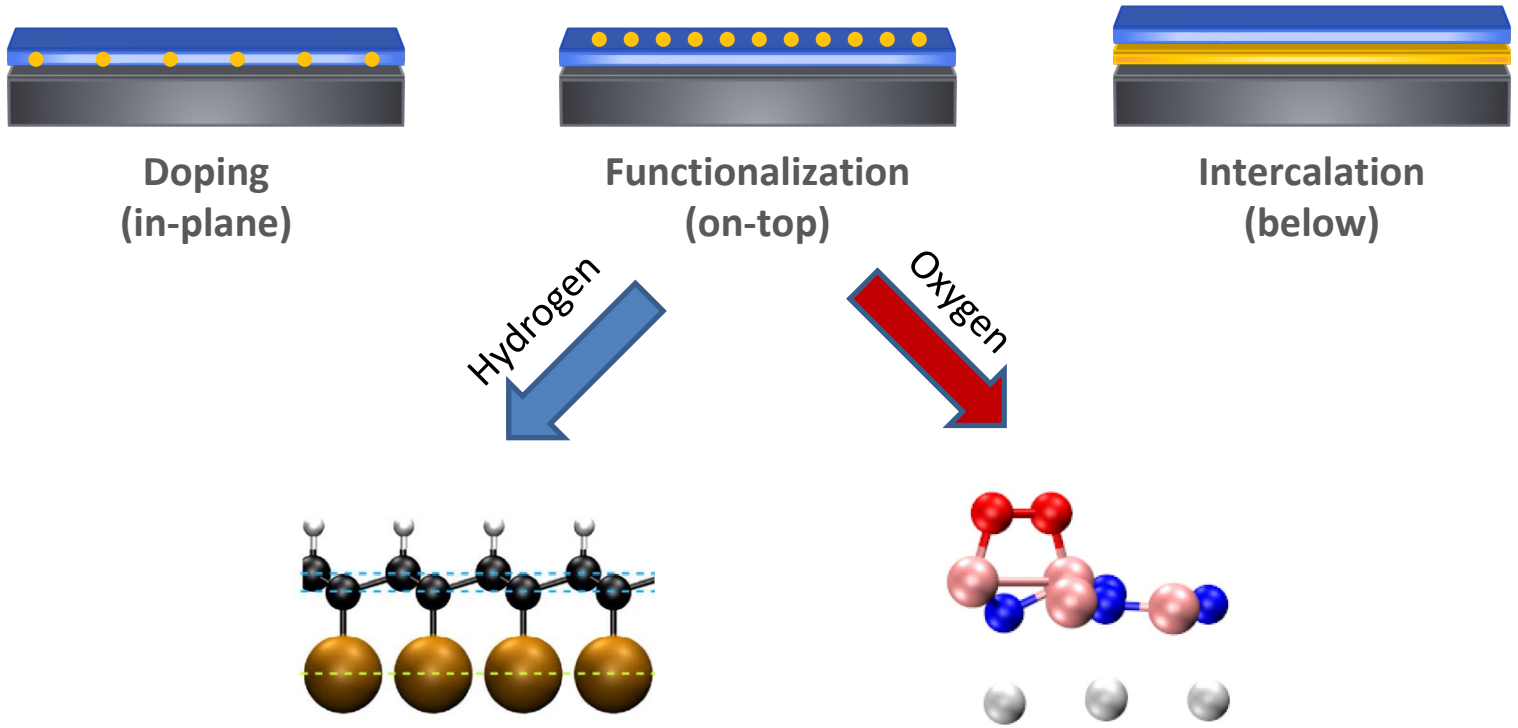
## Chemical analysis

→ Materials properties

# Chemical modification of 2D materials

**How can we tailor the properties of 2D materials with respect to specific applications?**

→ Chemical modification



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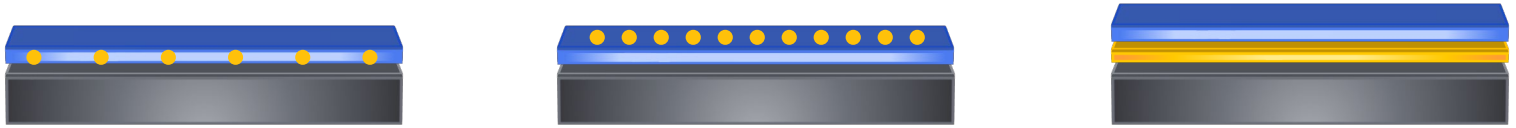
→ Chemical modification



Doping
(in-plane)

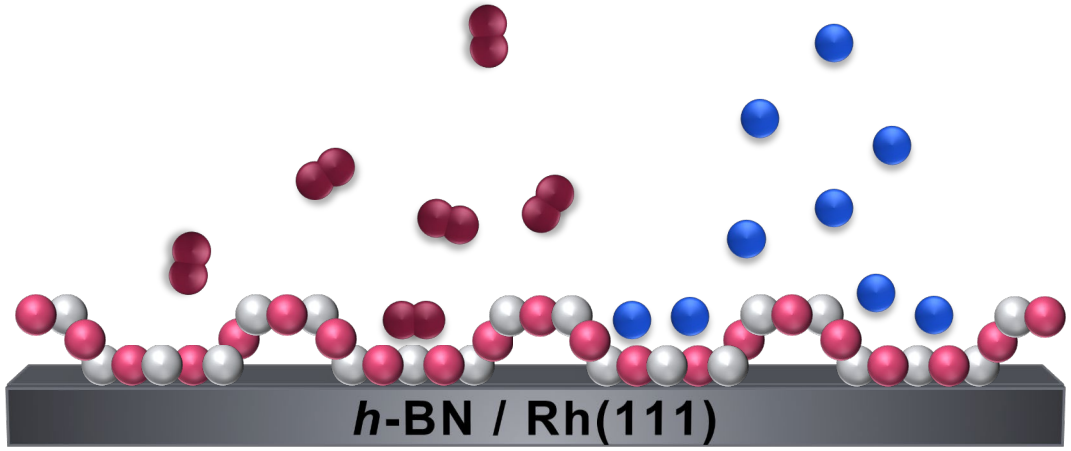
Functionalization
(on-top)

Intercalation
(below)

**How can we achieve spatially controlled chemical modification?**

→ Moiré as template

- Different reactivity of pores and wires = key to selectivity
- Hydrogen and oxygen



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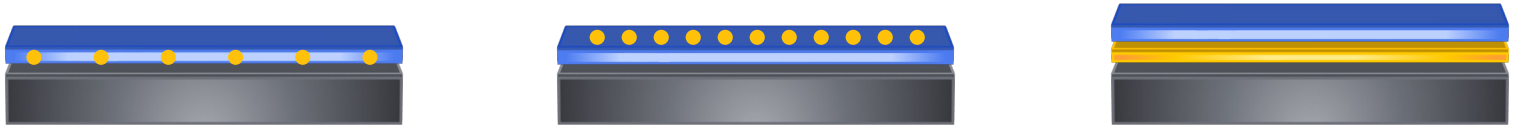


Doping
(in-plane)

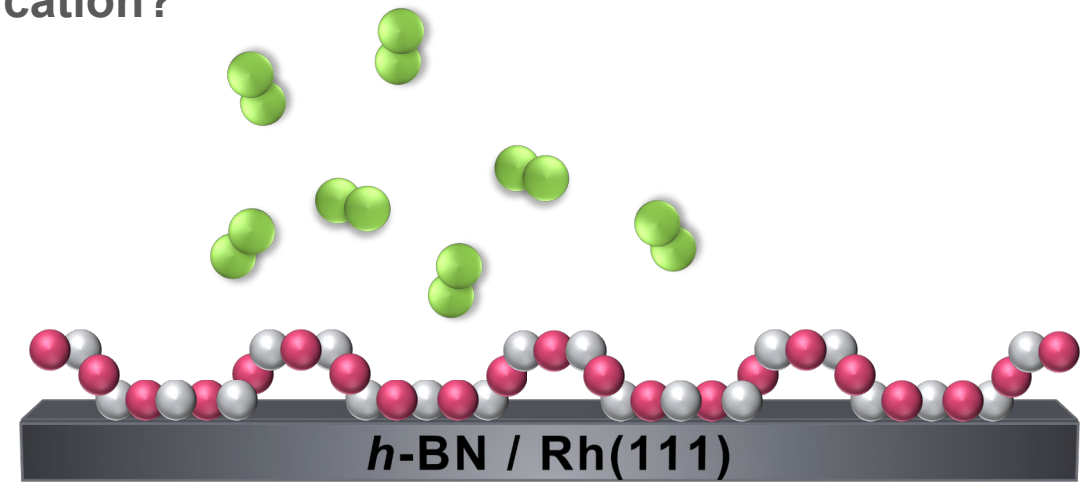
Functionalization
(on-top)

Intercalation
(below)

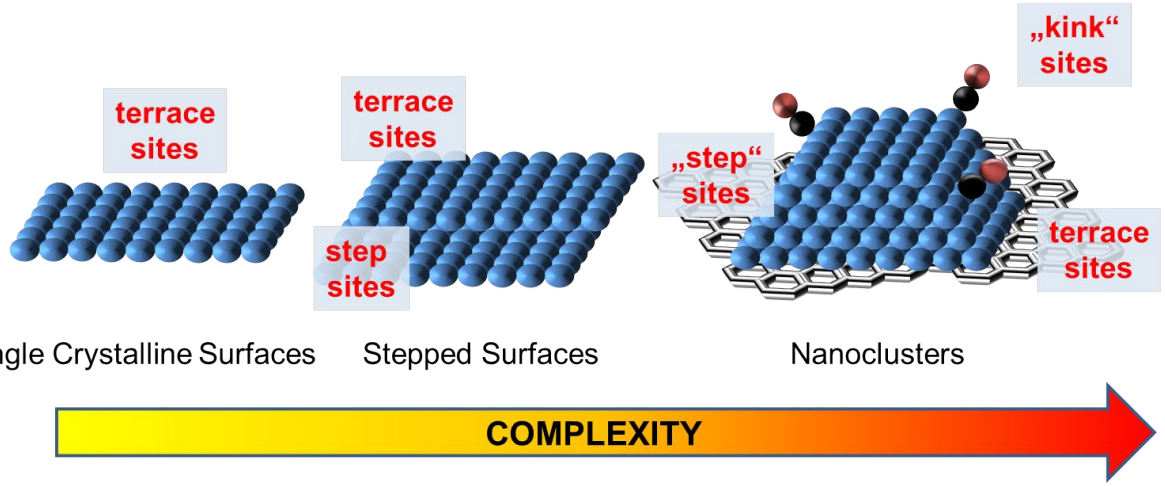
**How can we achieve spatially controlled chemical modification?**

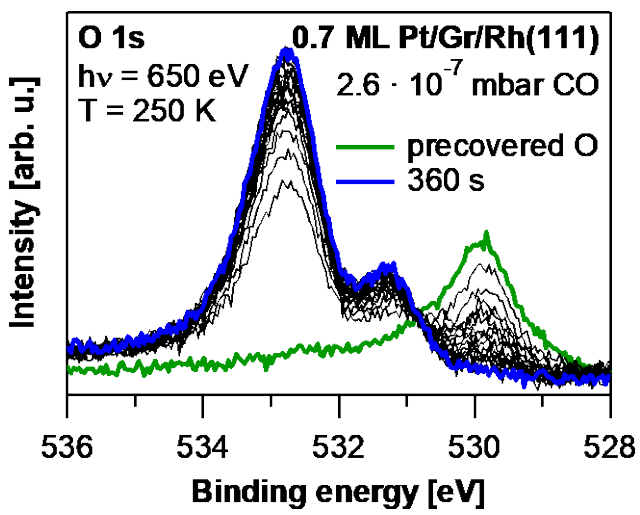
→ Moiré as template

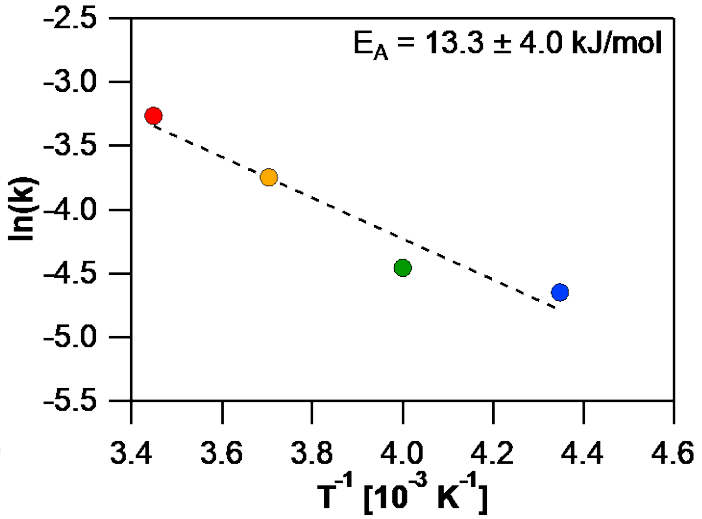
- Different reactivity of pores and wires = key to selectivity
- Hydrogen and oxygen
- Halogens → Bromine

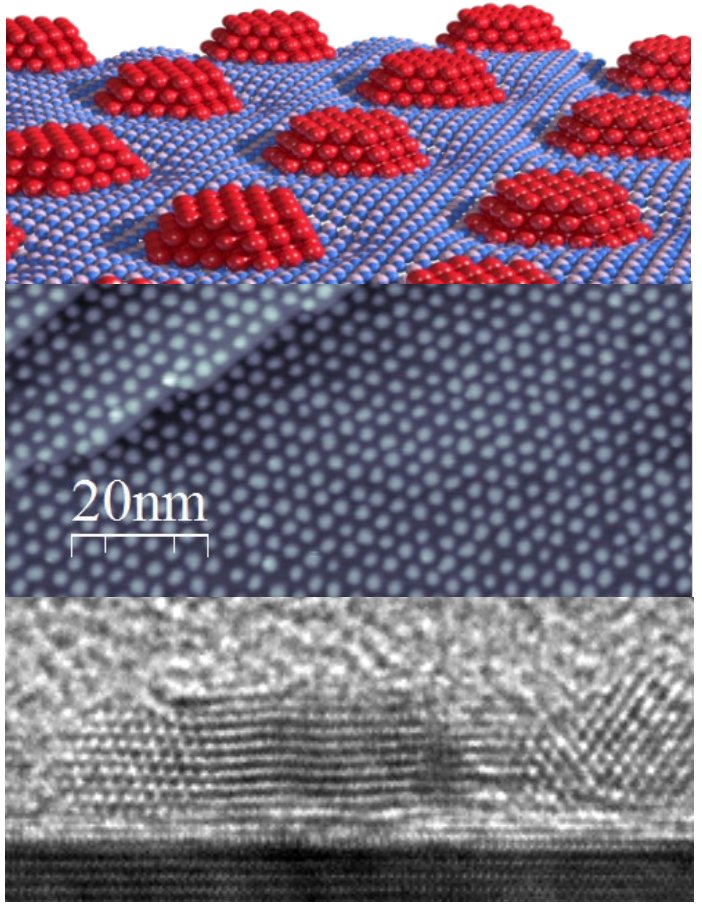


# Fundamental insights in surface reactions
# From flat surfaces to nanoclusters



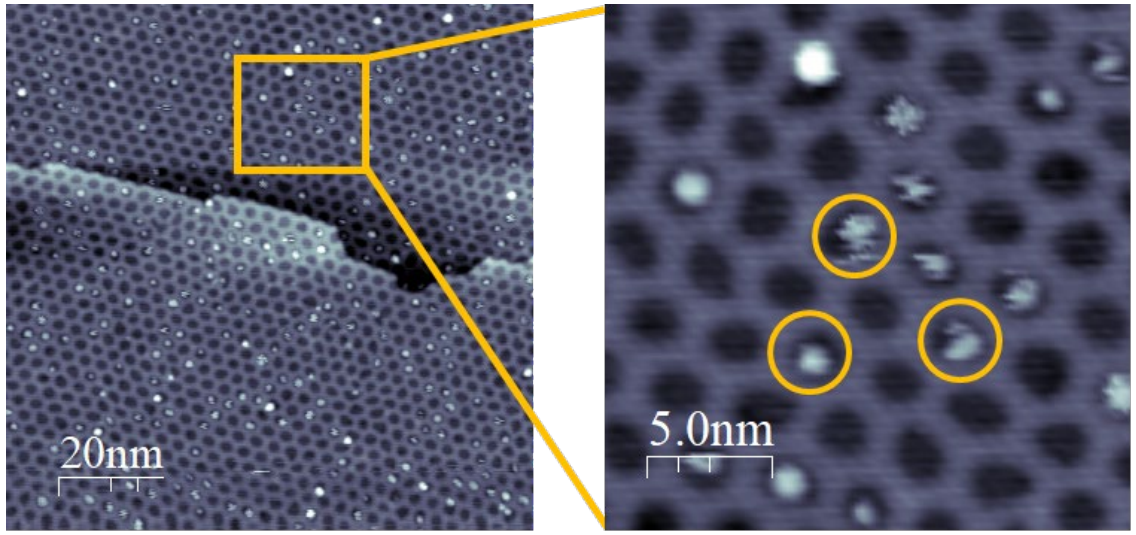



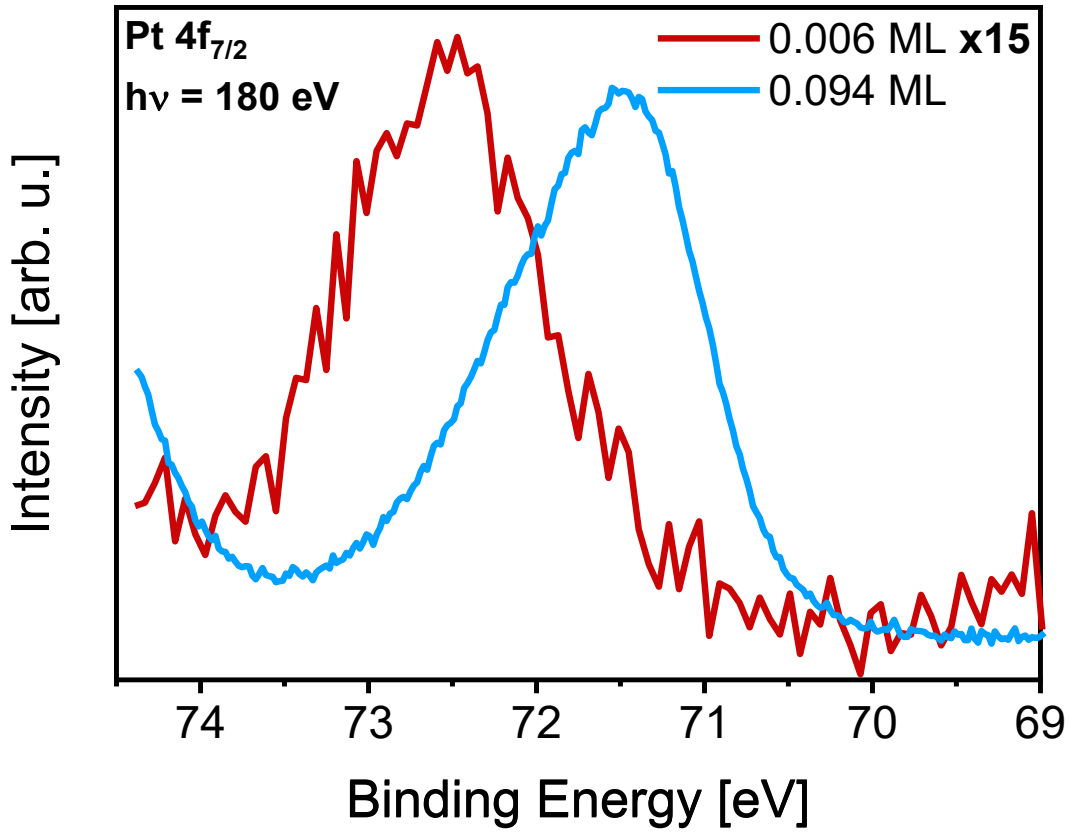

Ordered nanocluster arrays on 2D materials
→ Reaction on nanoclusters


Papp, Catal. Lett. 147 (2017) 2.
Düll, Papp, Phys. Chem. Chem. Phys. 21 (2019) 21287.

# Spectroscopy of small clusters




*Average size 1.7 atoms* *Single Pt atoms*




Low coverage (0.005 ML)

- 2D gas phase in pores
- Stable over extended time

➔ Spectroscopy (Chemical information)

➔ Clusters

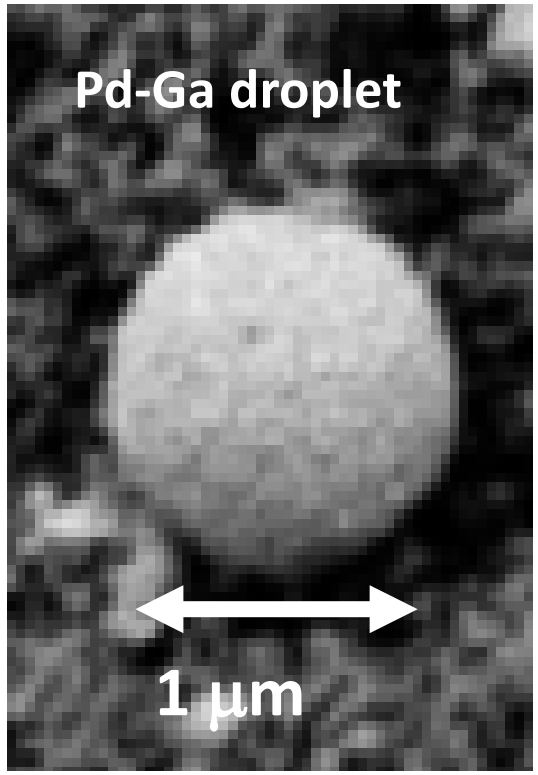
➔ Single Atoms

**➔ Size dependent catalysis**

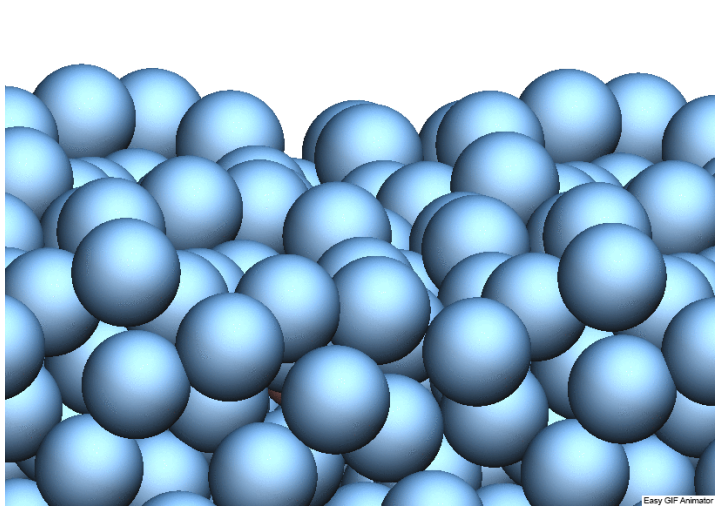
**➔ Single atoms for chemistry under controlled conditions**

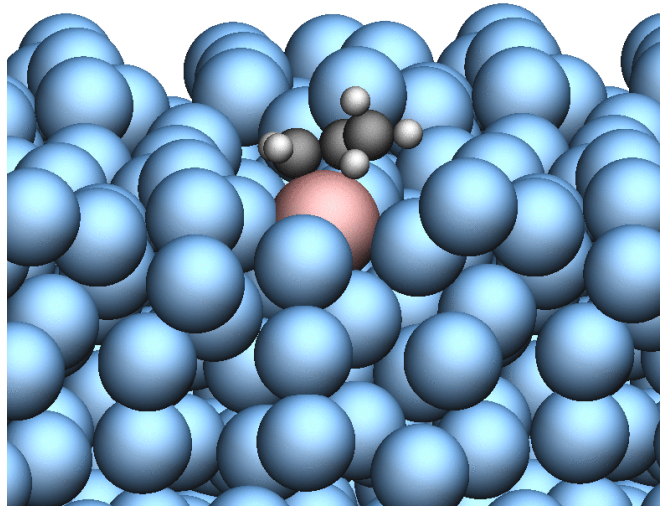
Düll, et int., **Papp** Phys. Chem. Chem. Phys. 21 (2019) 21287

# Supported Catalytically Active Liquid Metal Solutions




**Highly dynamic surface**
**Active site:**
**Single Pd atom dynamically appearing at interface**





**Ab initio molecular dynamics simulation**
**Görling et al.**

# Summary

- Model catalysis and surface science studies
  - from flat surfaces to nanoclusters
- 2D Materials
  - growth
  - Modification
- Single Atom Catalysis
  - liquid metal catalysts
- Energy storage
  - LOHC (Liquid Organic Hydrogen Carriers)
  - strained molecules