Aalto University

# CHEM-E5145
# Material Substitution

Workshop 4

31.1.2019

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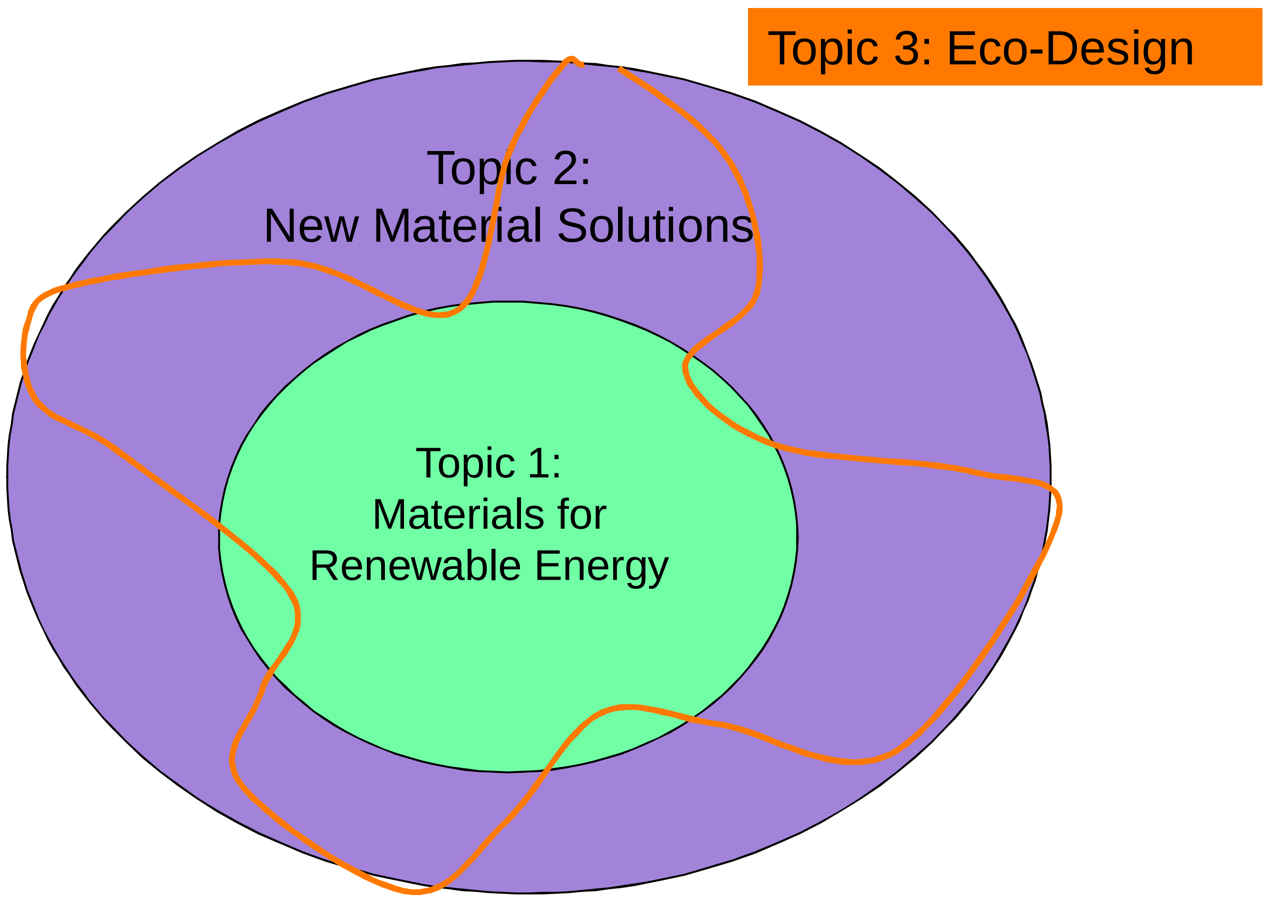
# Indentent learning outcomes Workshop IV

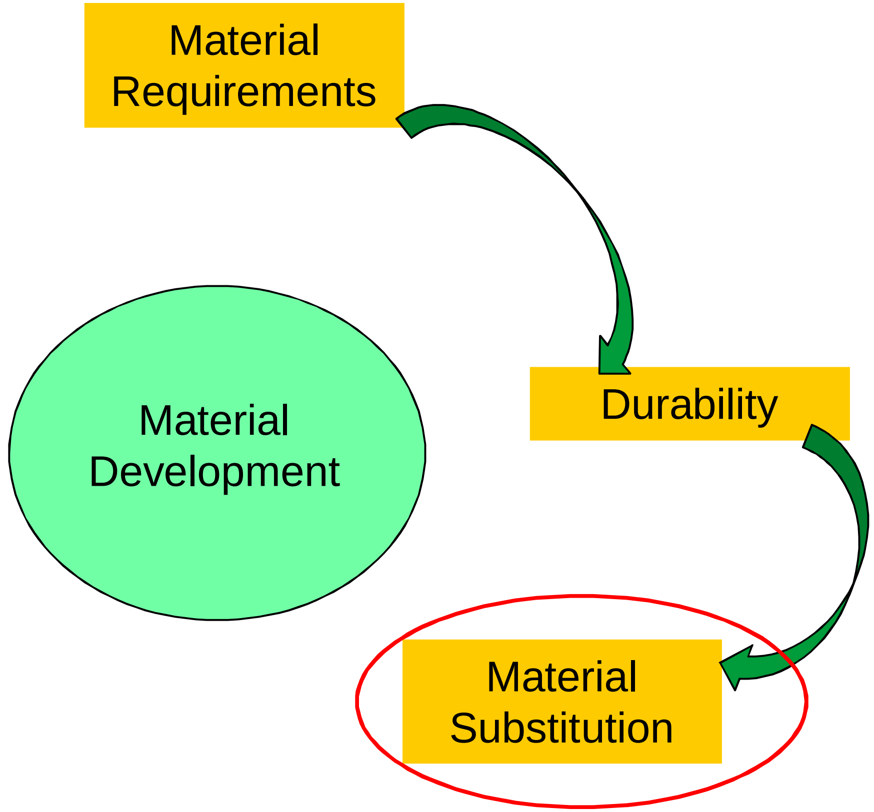
Identify common degradetion mechanisms in these applications

Share the expertise of ones field in a heterogenius team

Recognition why new material substitution is challenging → Develop new material solutions and eco-designs


Topic 3: Eco-Design
Topic 2:
New Material Solutions
Topic 1:
Materials for
Renewable Energy

# Topic 2 – New Materials Solutions



# Workshop timetable

- 8.30-9.30 poster preparation
- 9.30-10 gallery walk with posters
- 10-10.15 Sum-up the posters

  Break 15 min.

Workshop atmosphere 2016

- 10.30-11.00 Material substitution lecture
- 11-11.15 Task 3 info + new groups
- 11.15- 11.45 Peer-review of Flip reports + videos preparation

# Workshop IV - Poster

**The poster should include:**

What are the most relevant durability issues in your application?

What is the time frame of “durability” in your application?

How could the durability be enhanced?

Visualization –
to support understanding

# Flip Activity

- Poster tour
  - > Each of you will have your own team and you will teach the topic to others (5 min /poster)
  - Make questions, what did you not understand! (if not don't know – ask teacher or make a post-it tag to the poster

- Poster's and their presenting is evaluated
  - You all vote for the best poster (clear message)
  - The best poster, get's automatically 4 p./workshop
  - Others get evaluated by the teacher 0-4 p.

# Best Poster selection

Vote for the best poster!

# Sum up from the poster's

What were the most common critical degradation in these applications?

# Brainstorm in your group

Any new angle from the durability issues that you might use in your New Material Solutions

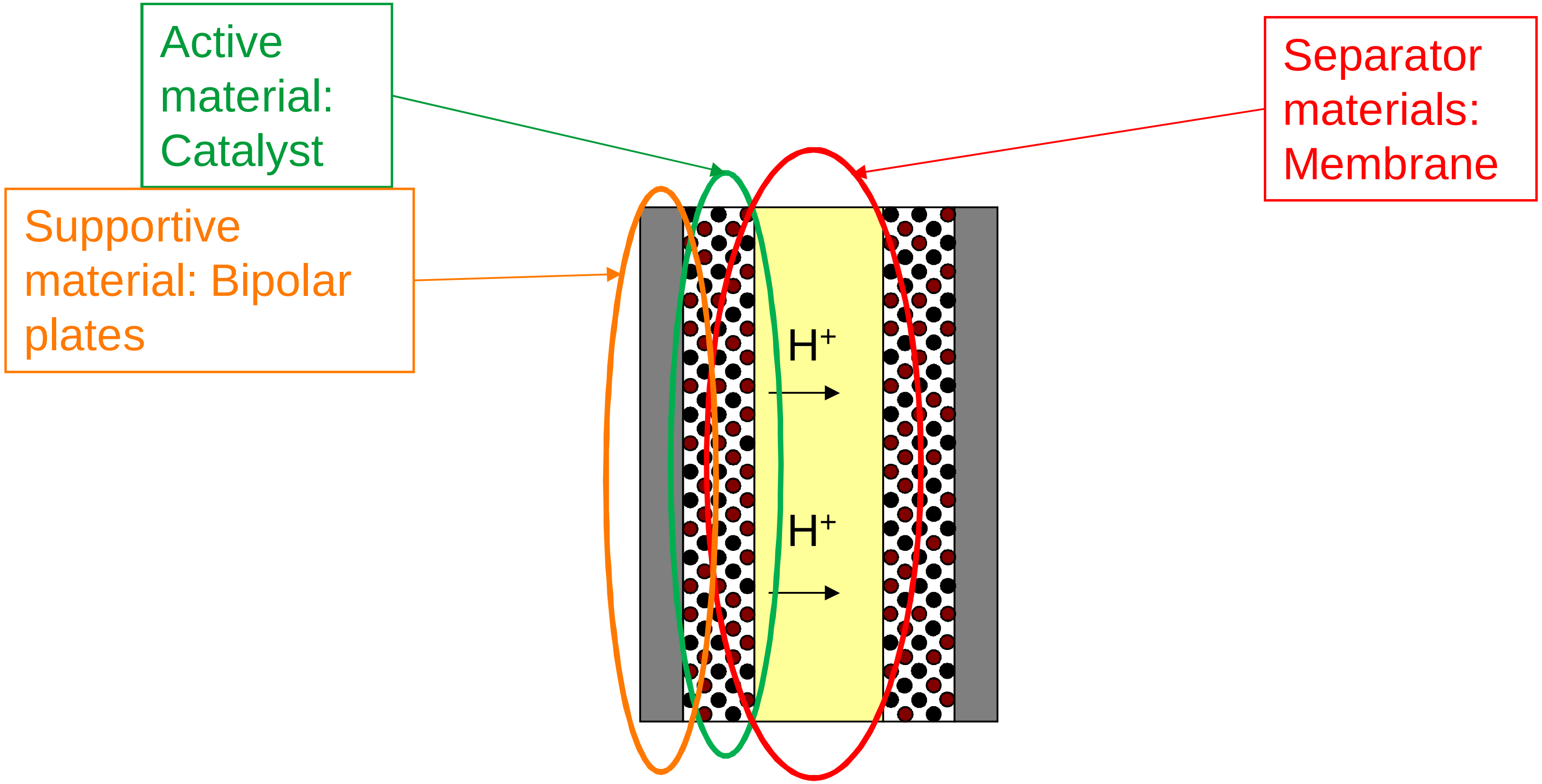
New Material Solution

# Break 15 min.

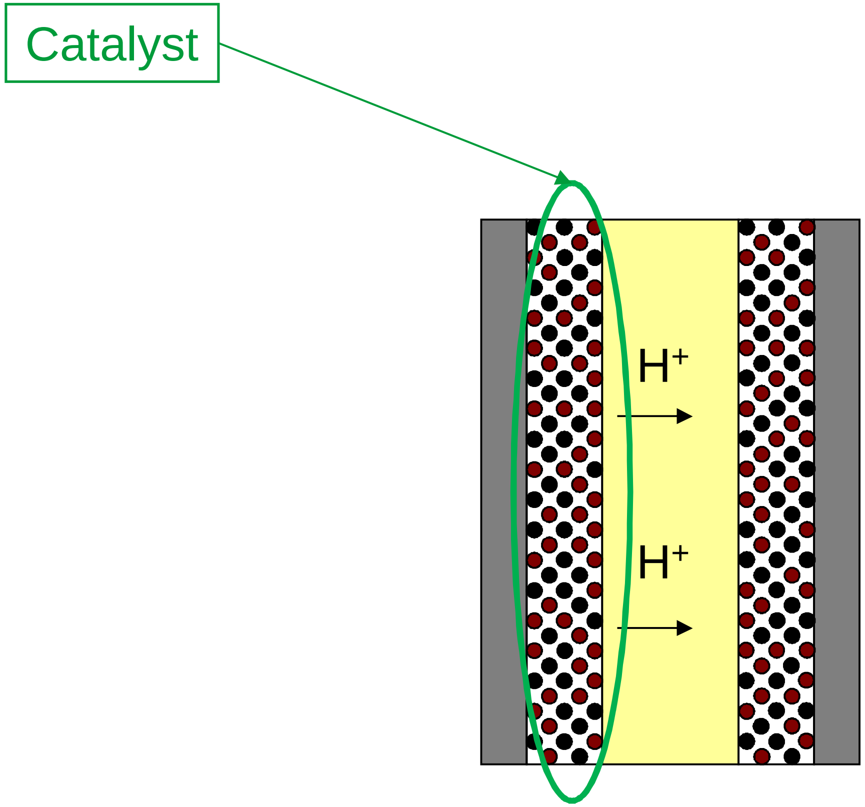
# Material Substitution

Why have we selected problematic materials for the active materials?

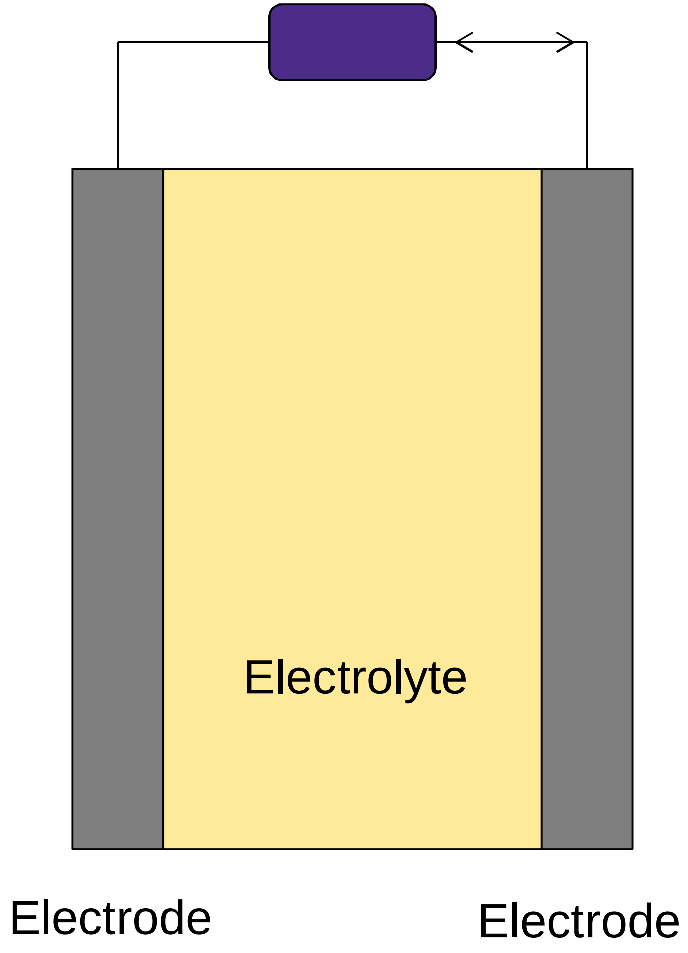
# Different components



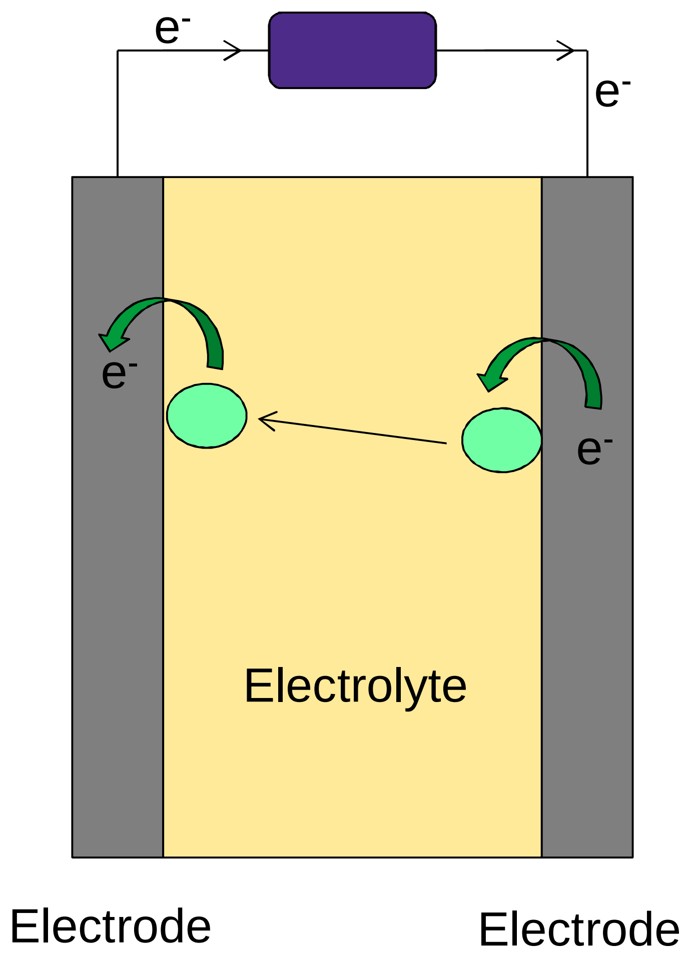
# Substitution – Active Materials



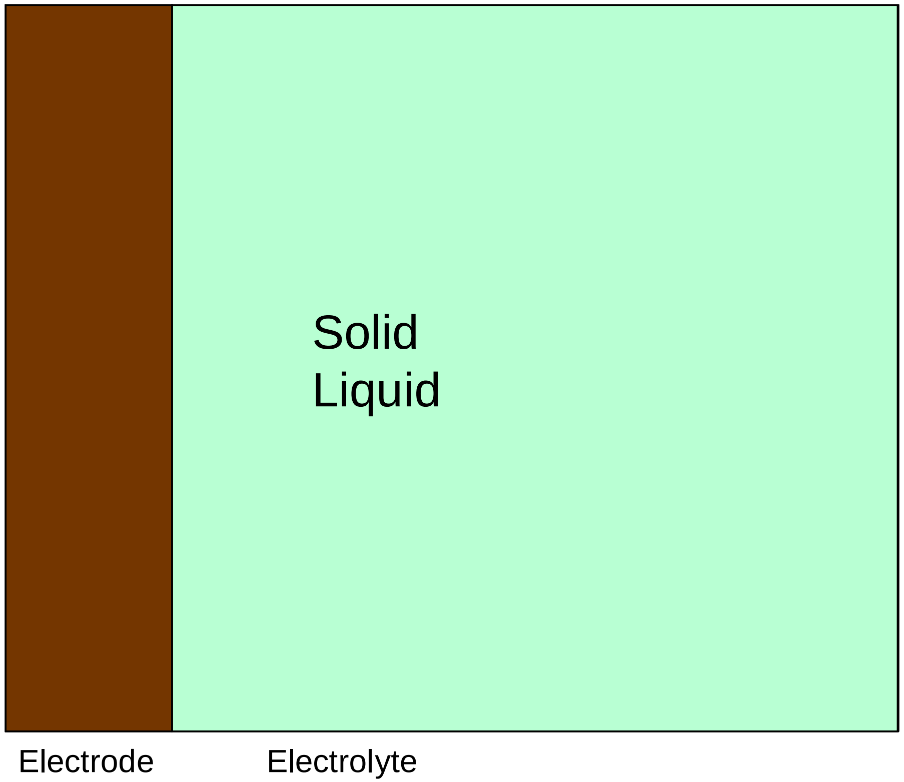
# Electrochemical device



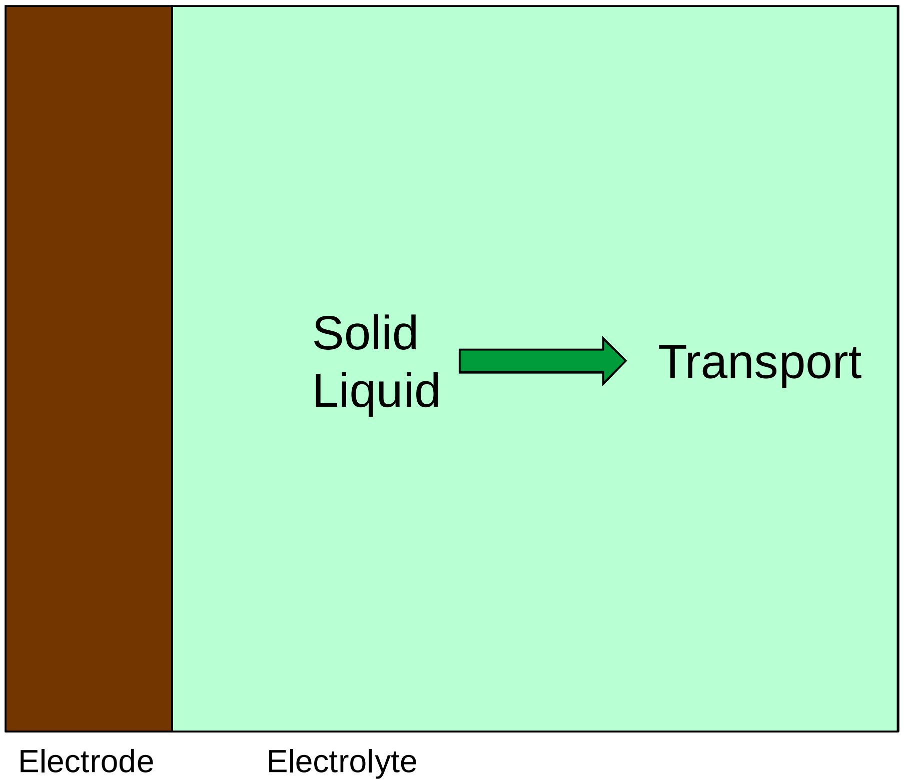
# Electrochemical device



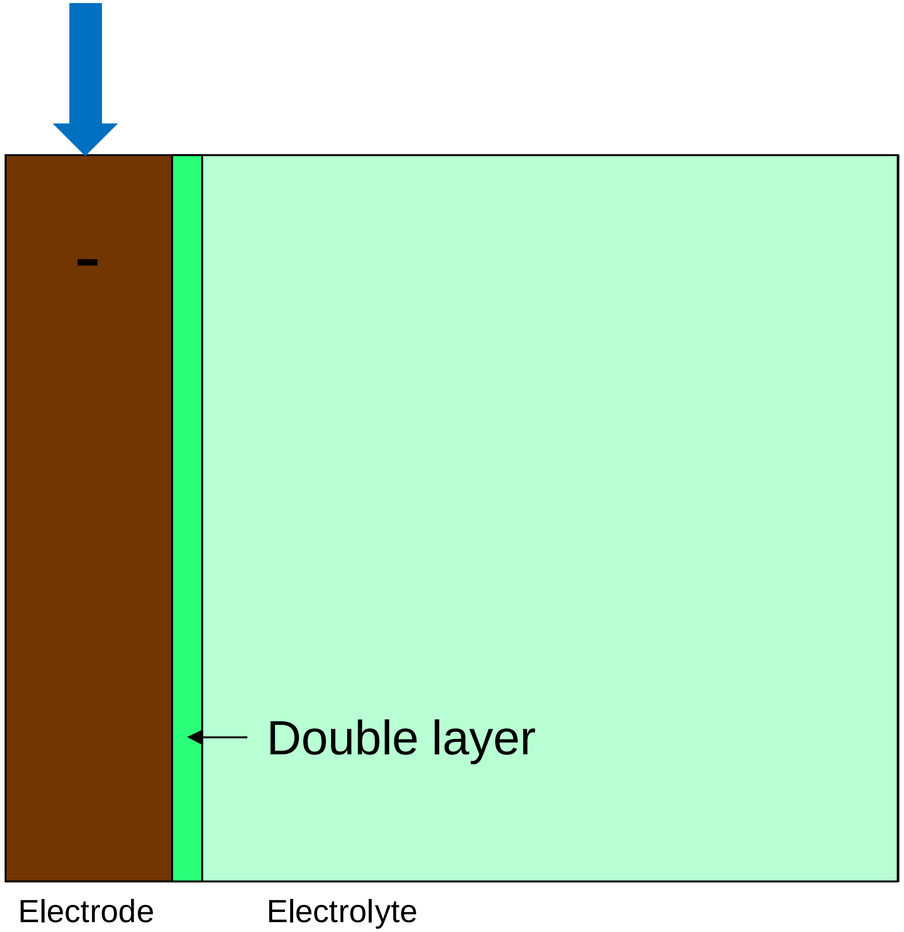
# Reaction on two phase boundary



# Reaction on two phase boundary

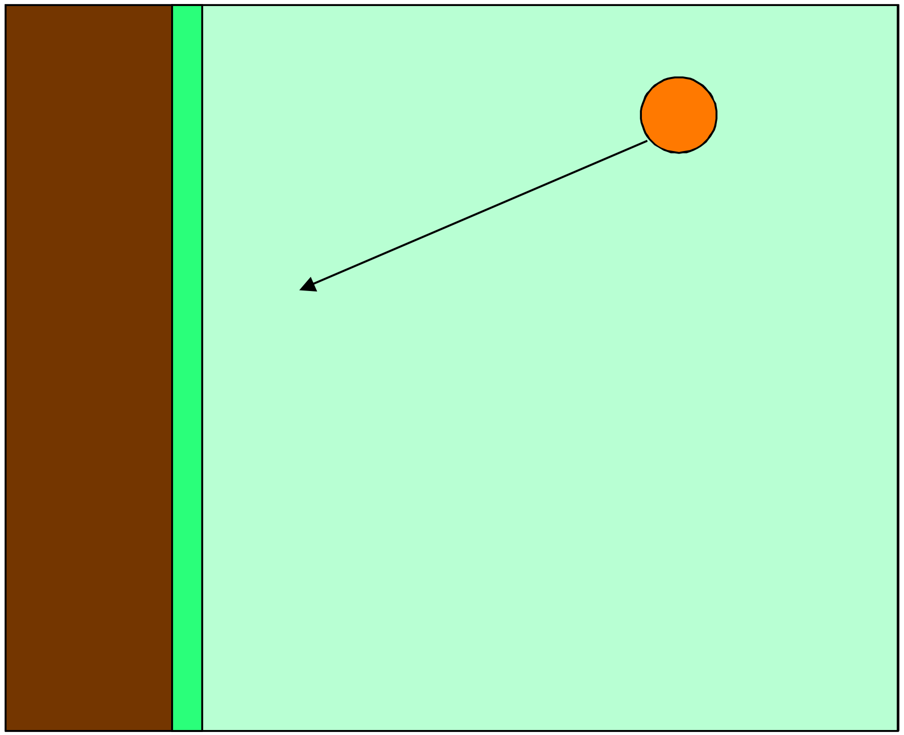


# When potential is applied



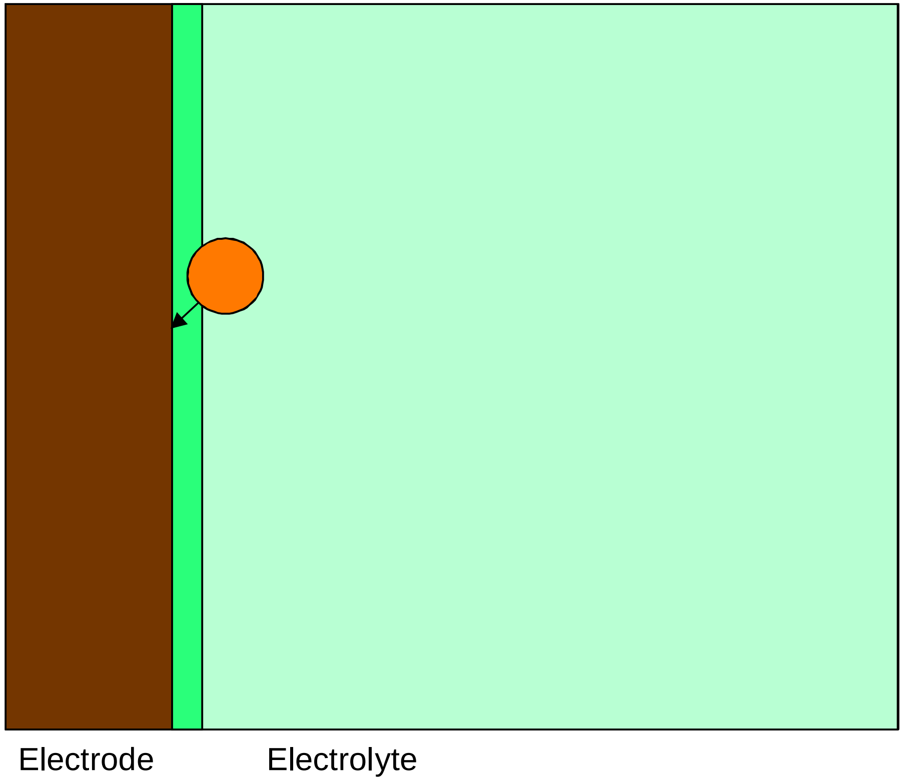

Ions in the electrolyte (if liquid) will organize to the electrode surface and create a Double Layer

# Reaction on two phase boundary



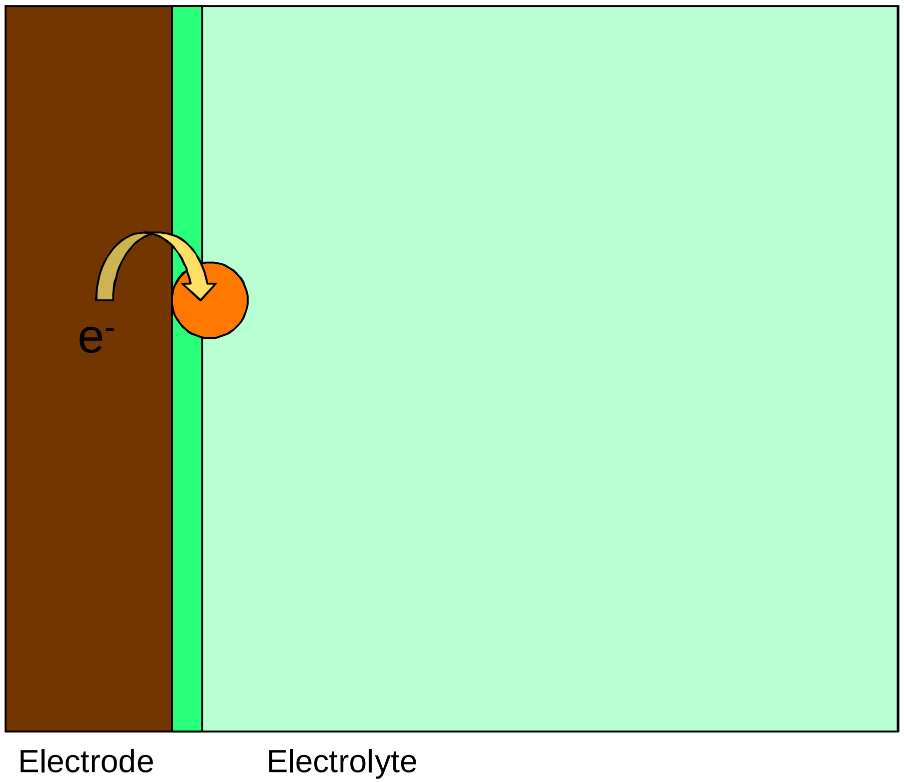

Diffusion
vicinity of the electrode

# Reaction on two phase boundary



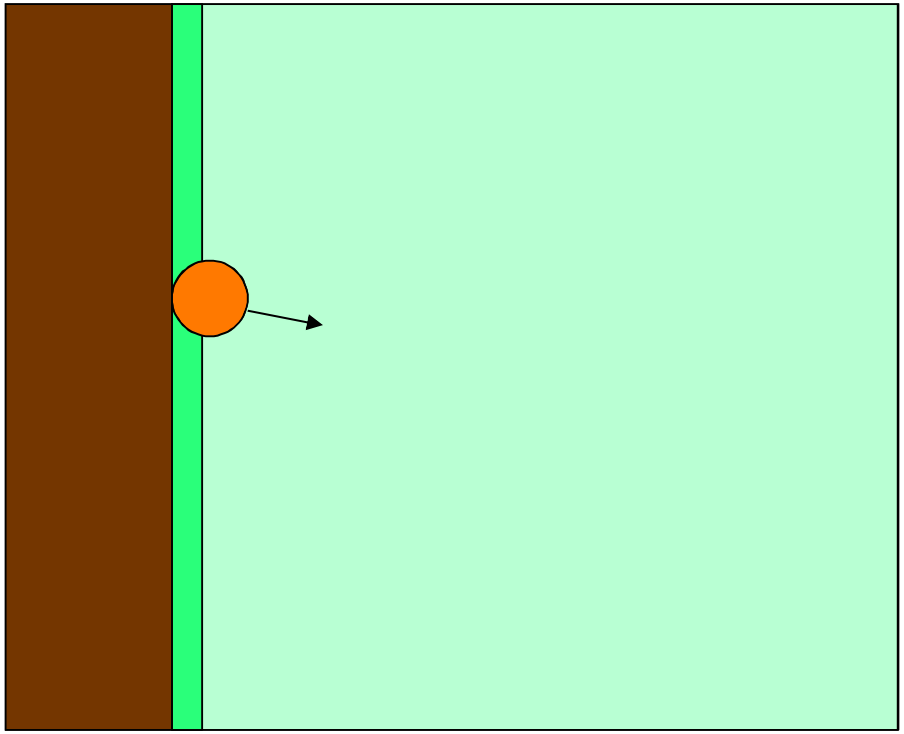

Adsorption
to the electrode

# Reaction on two phase boundary



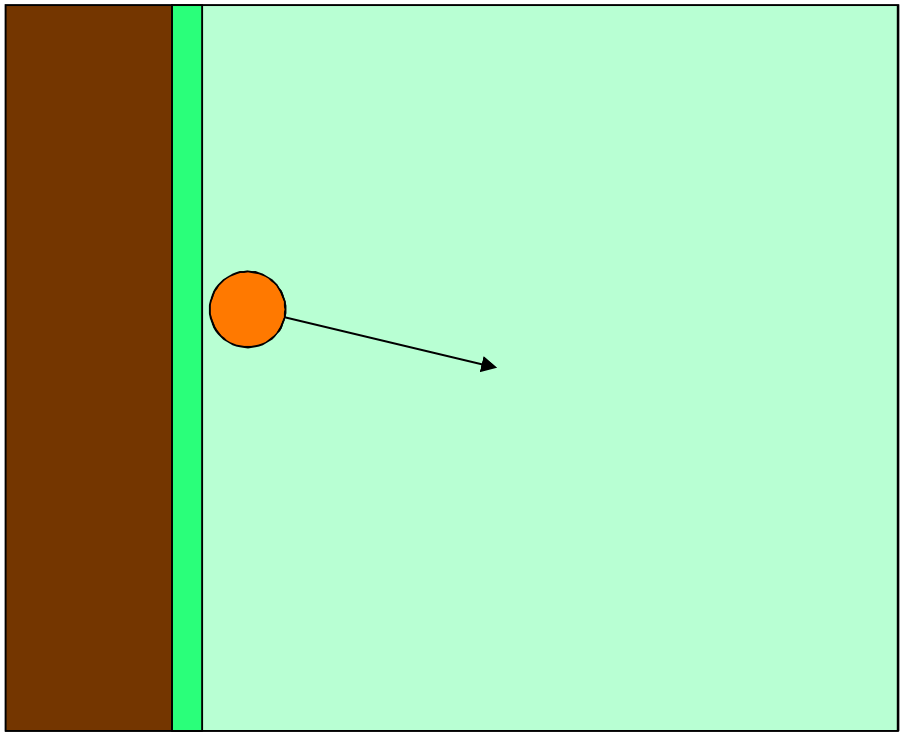

Reaction:
electron transfer

# Reaction on two phase boundary




Desorption
From the electrode

# Reaction on two phase boundary




Diffusion
Back to the bulk

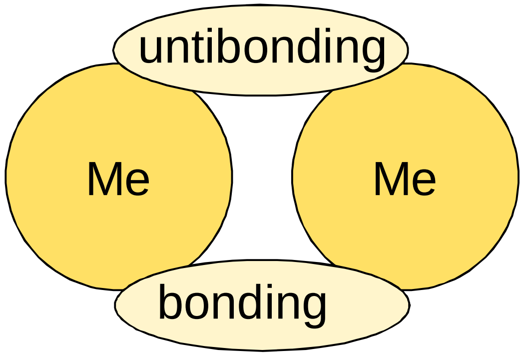
# Active material: Catalyst

What is a catalyst?

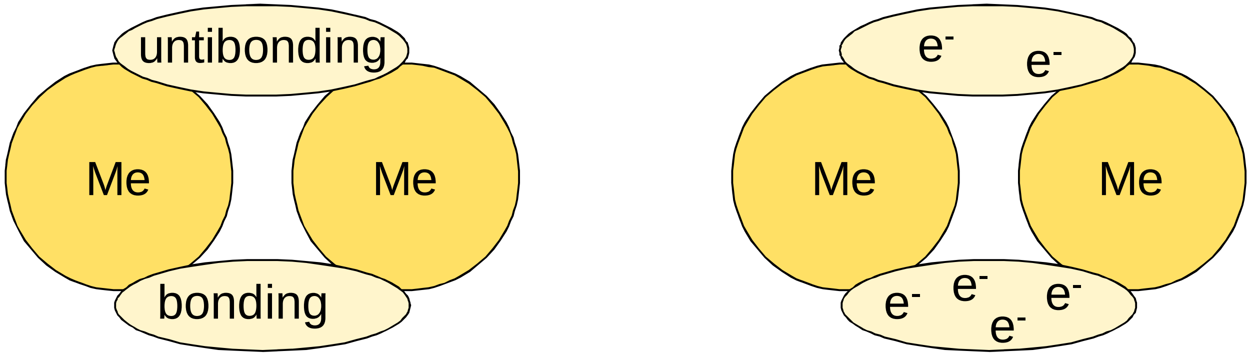
Electrocatalyst?

A material working a catalyst in a reaction involving an electron transfer.

# Metal atoms



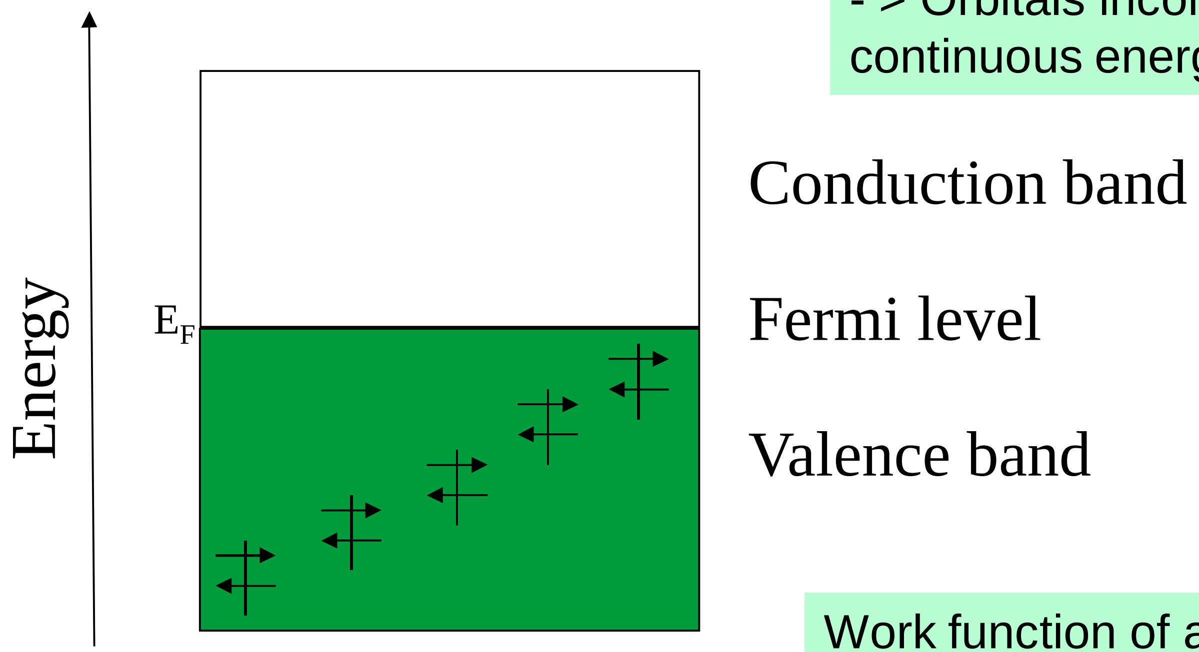
# Metal atoms




If there are more electrons on the bonding orbital – the bond is stable

# Metal electrode

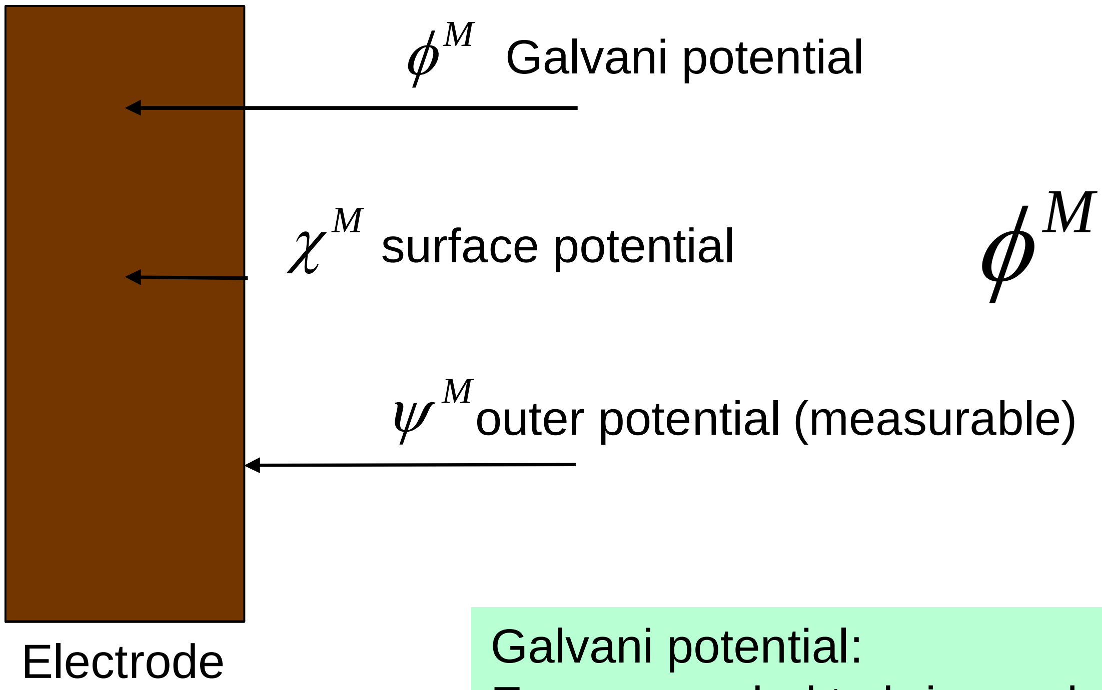
Formed of many metal atoms
- > Orbitals incorporate to continuous energy bands




$$E_F^M = -\Phi^M = \tilde{\mu}_e^M$$

Work function of a uncharged metal: The electrical work needed to remove an electron from the Fermi level of the metal to vacuum

# Electrode potential




$$\phi^M = \chi^M + \psi^M$$

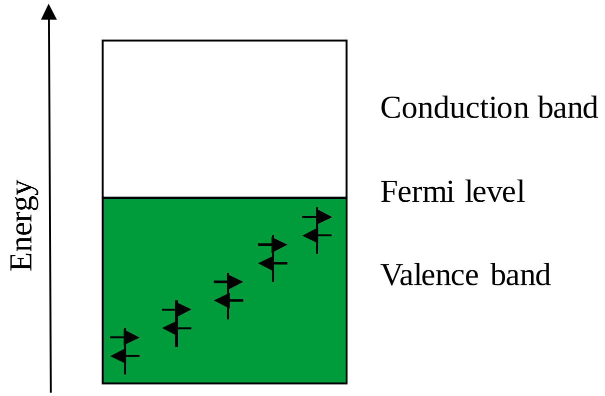
Galvani potential:
Energy needed to bring a charged particle from the vacuum to the inner part of the metal

# Metal electrode

$$E_F^M = -\Phi^M = \tilde{\mu}_e^M$$

Work function of uncharged electrode is?

$$\Phi^M =$$




Uncharged electrode

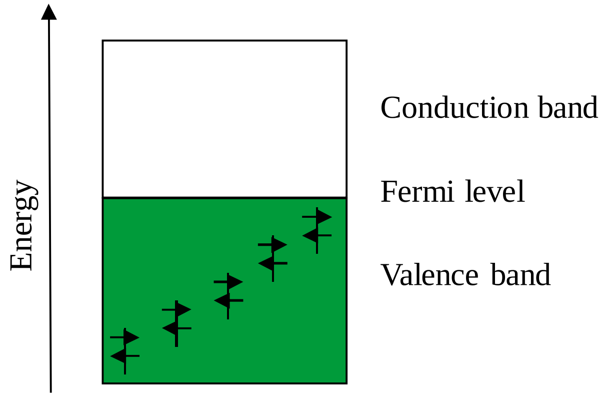
$$\tilde{\mu}_e^M = \mu_e^M - F\chi^M$$

# Metal electrode

$$E_F^M = -\Phi^M = \tilde{\mu}_e^M$$

Work function of uncharged electrode is

$$\Phi^M = F\chi^M - \mu_e^M$$




Uncharged electrode

$$\tilde{\mu}_e^M = \mu_e^M - F\chi^M$$

# Metal electrode

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Work function of uncharged electrode is

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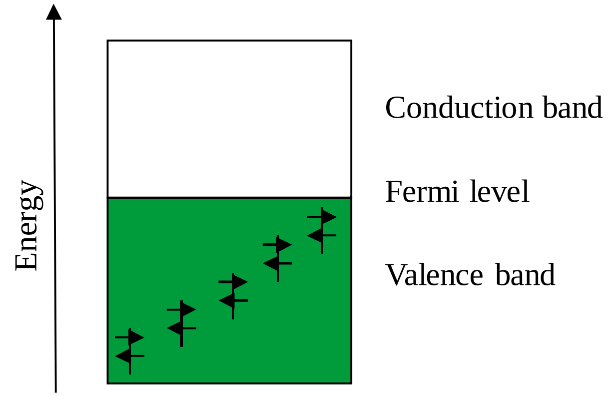


Uncharged electrode

$$\tilde{\mu}_e^M = \mu_e^M - F\chi^M$$

Work function of a metal effects

- Surface potential -> Adsoprtion of molecules on the electrode

# Work function

Work function of a metal effects

- Surface potential -> Adsoprtion of molecules on the electrode

$$\Phi^M = F\chi^M - \mu_e^M$$

Different metals

| | $\Phi$ (eV) |
|---|---|
| Pt | 6.35[1] |
| Au | 5.10[1] |
| Zn | 4.3[1] |

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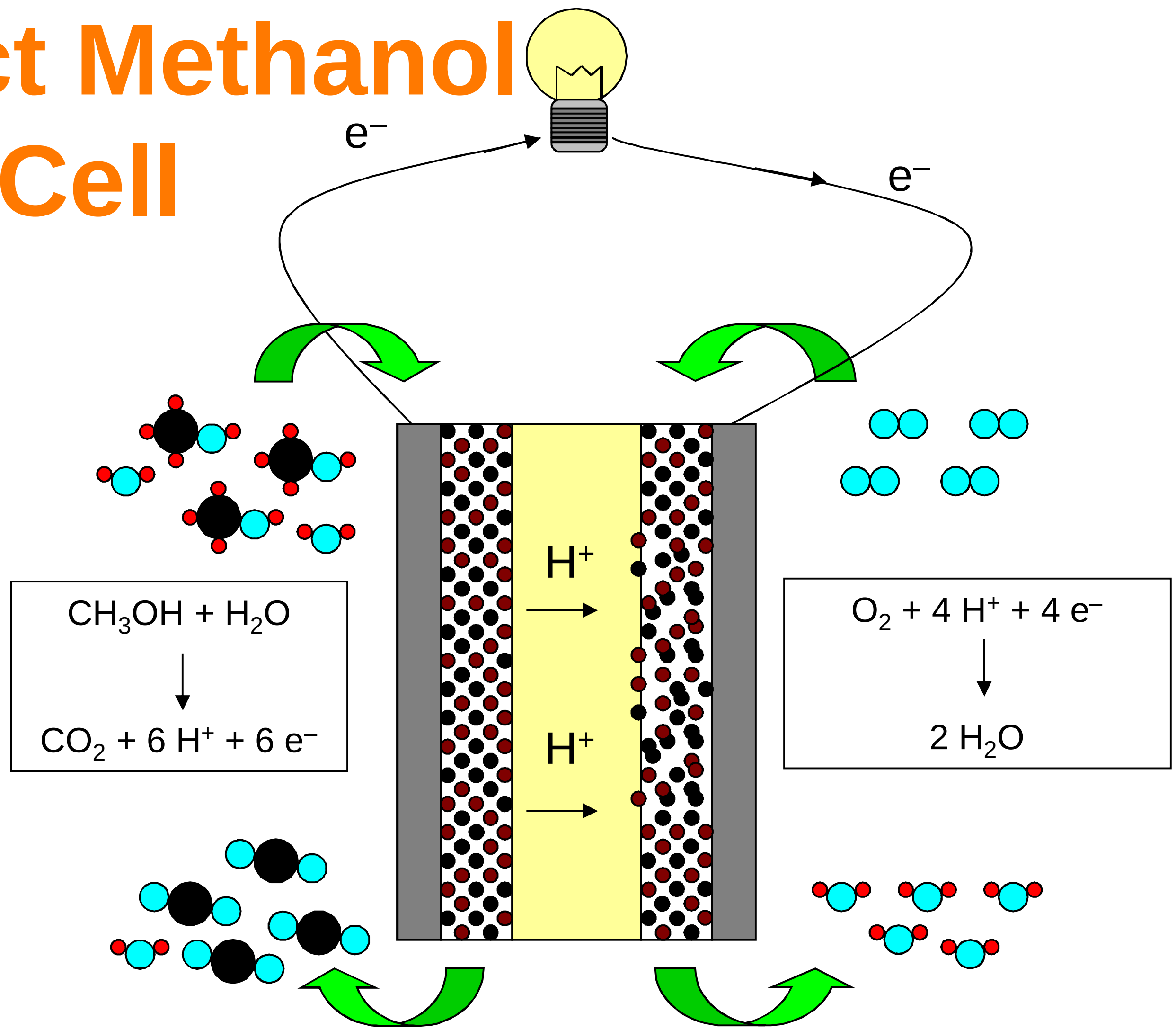
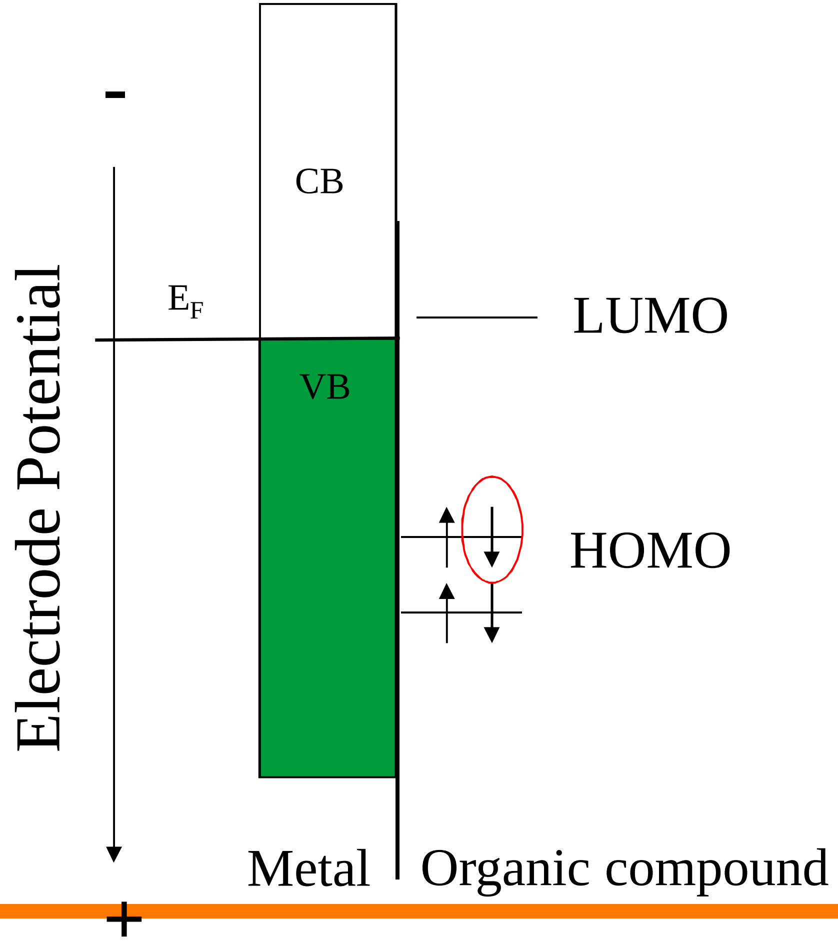
1) D. R. Lide (Ed.), CRC Handbook of Chemistry and Physics, 80th ed., CRC Press, Boca Raton 1999/2000.

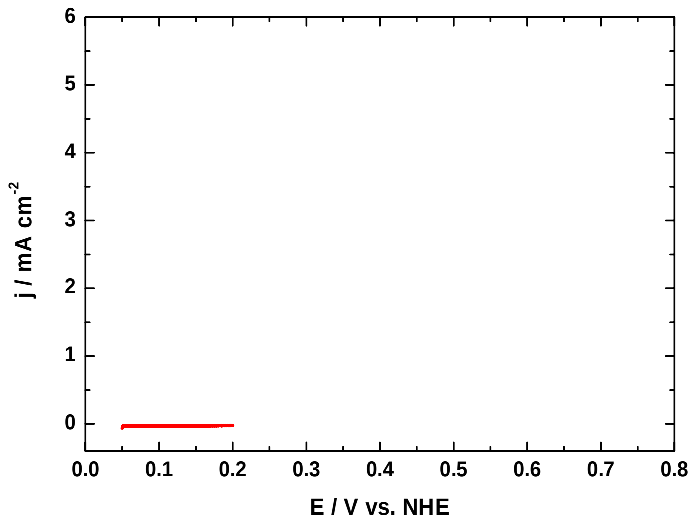
# Direct Methanol Fuel Cell




Total: $CH_3OH + 3/2\ O_2 \rightarrow CO_2 + 2\ H_2O$

# Electrooxidation of methanol



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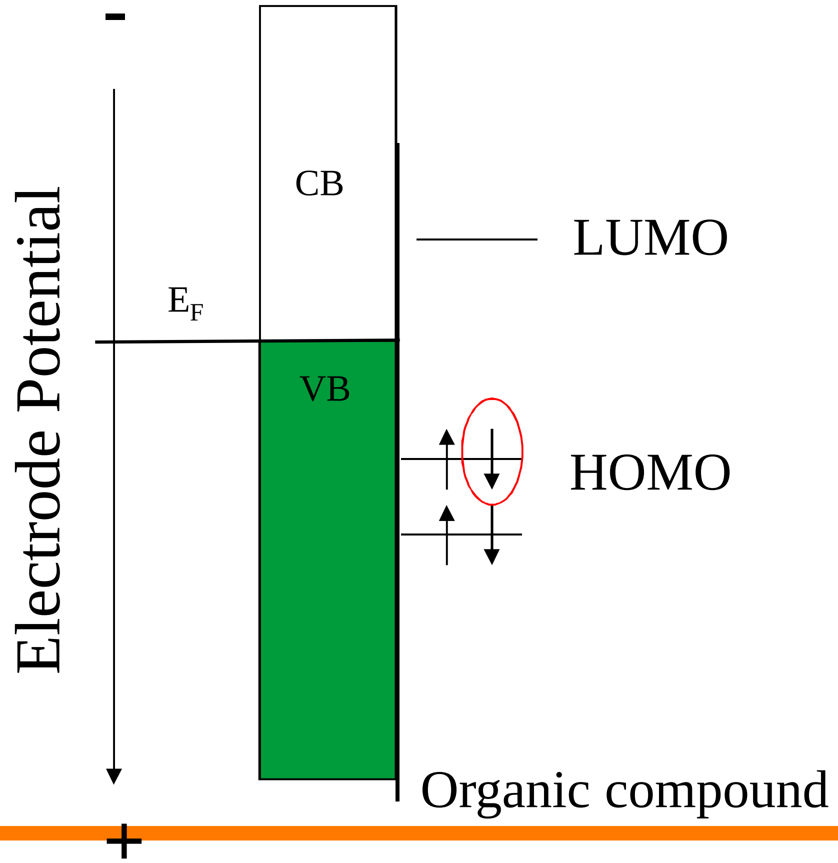


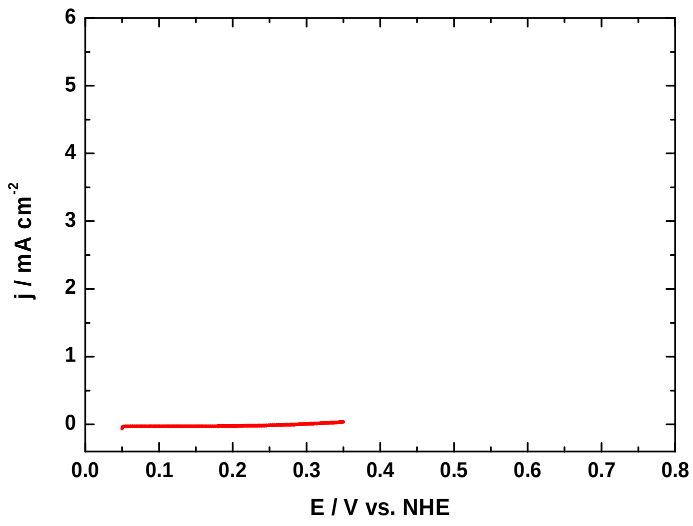

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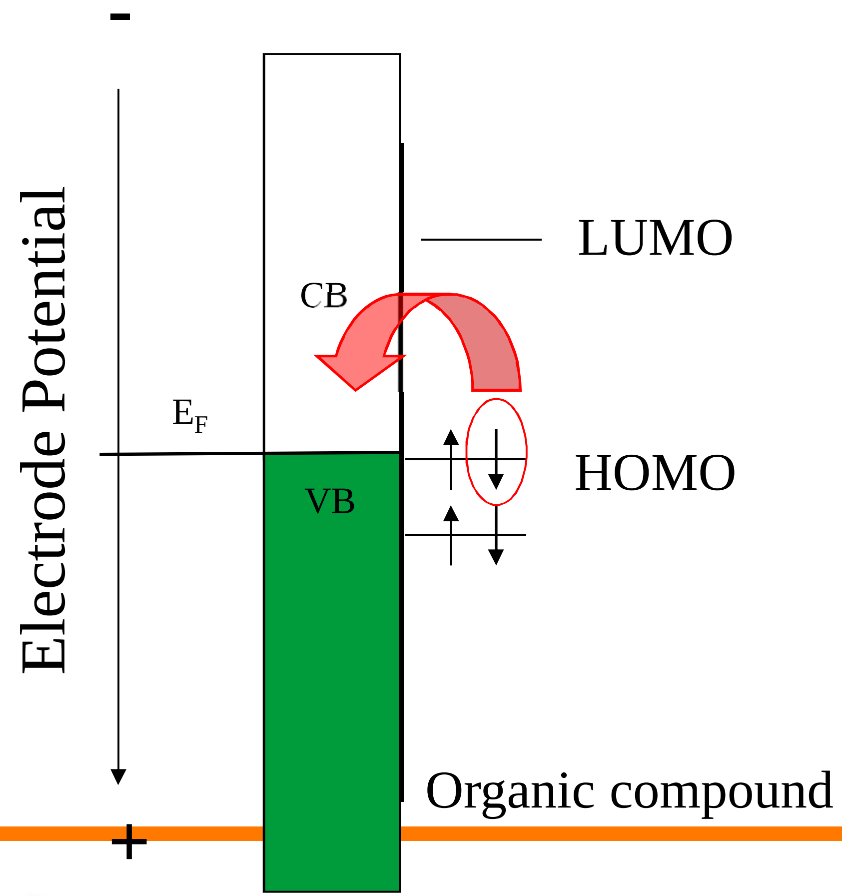


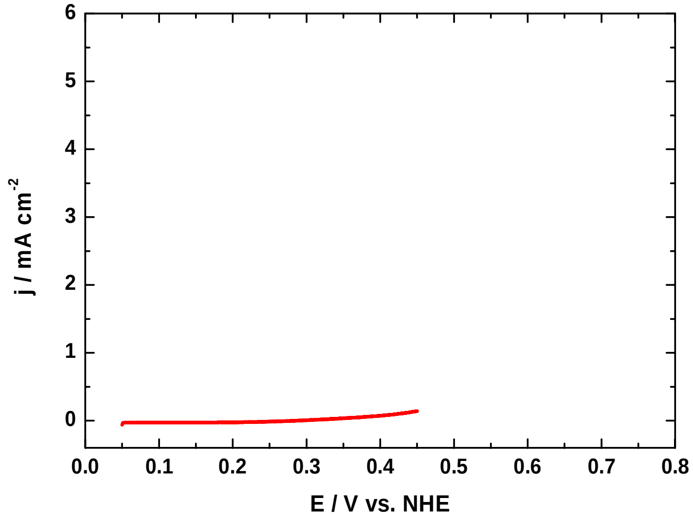

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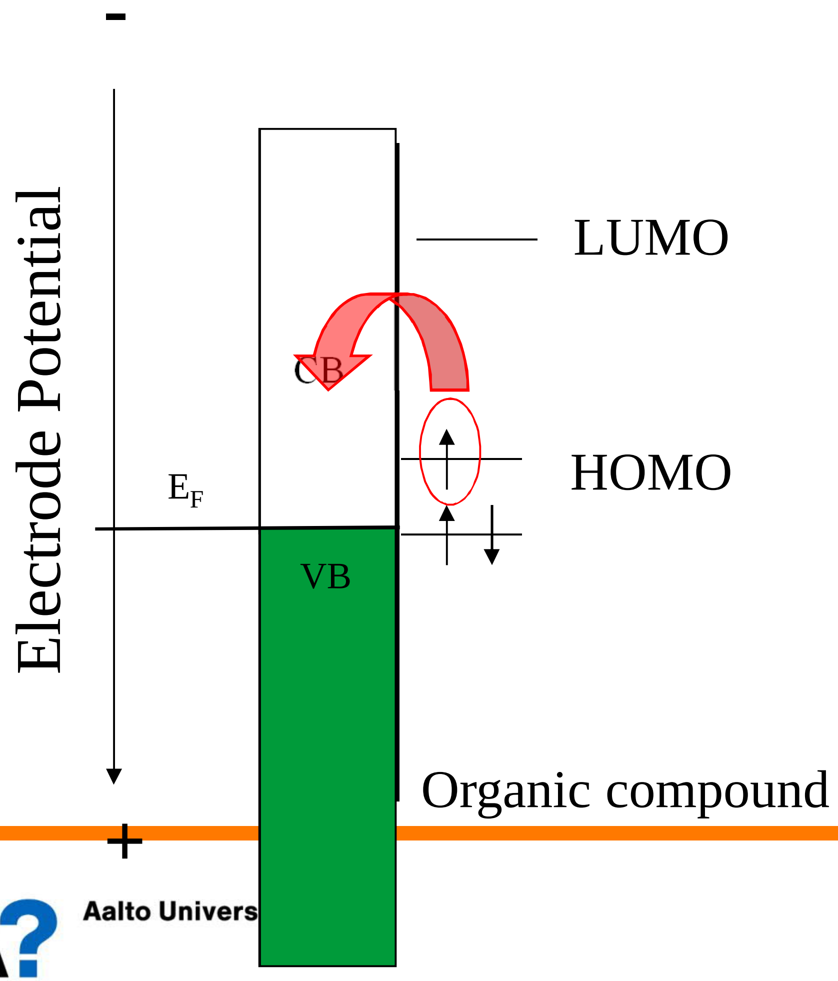


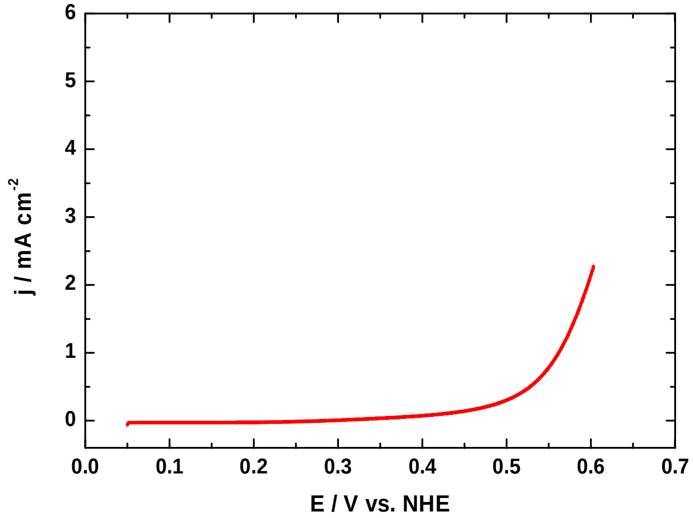

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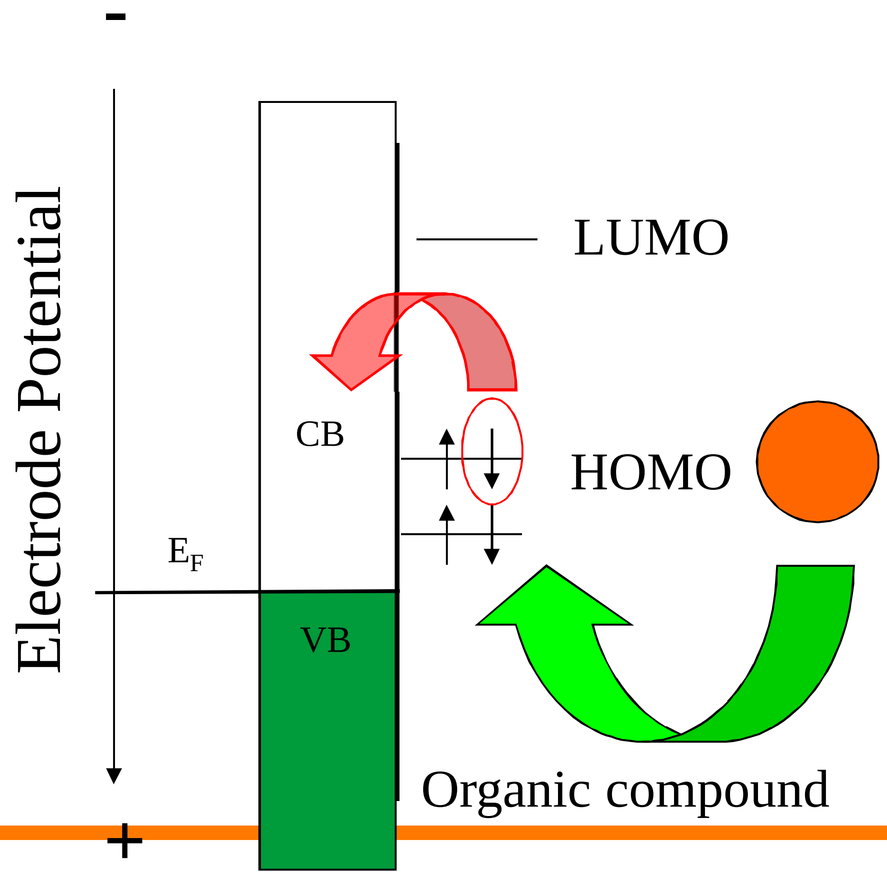
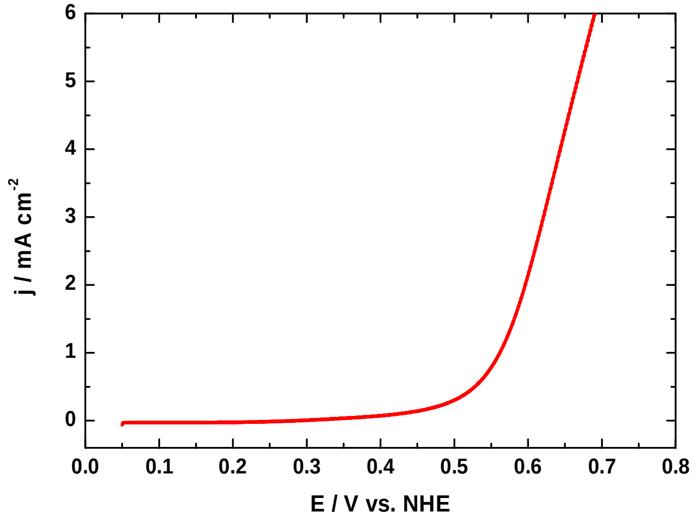
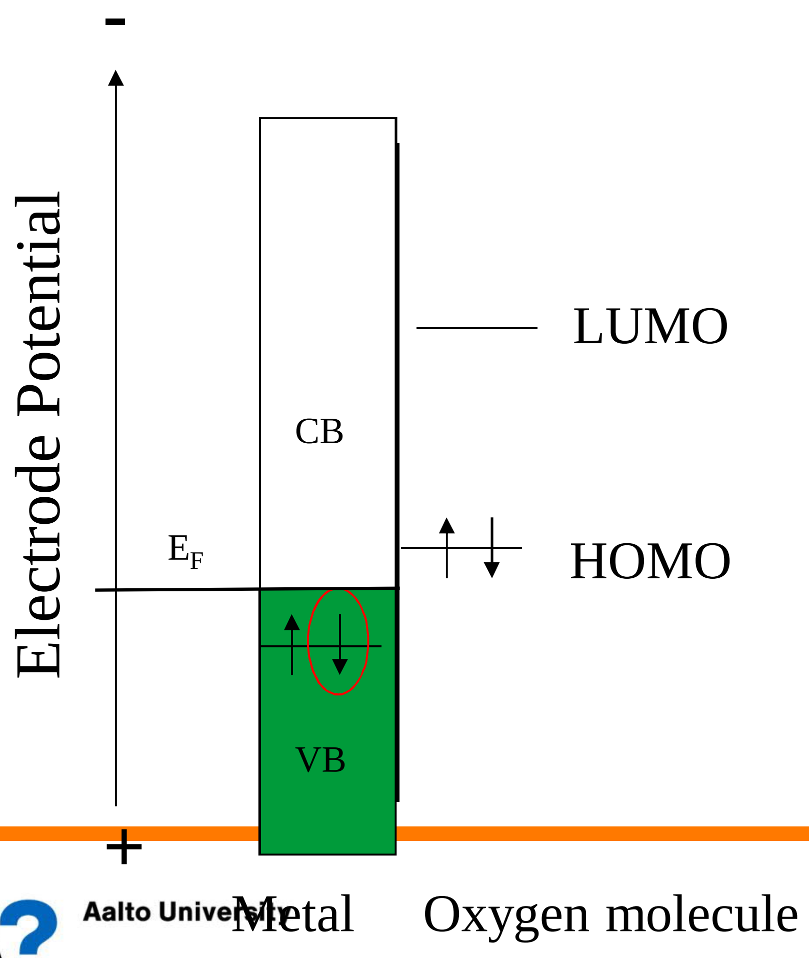
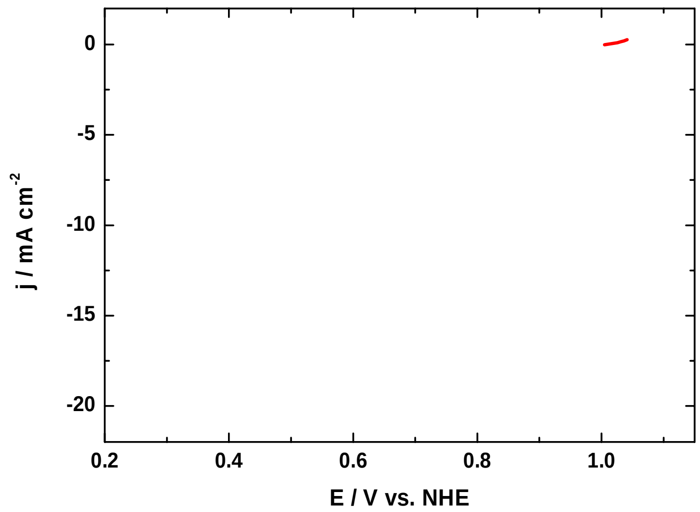


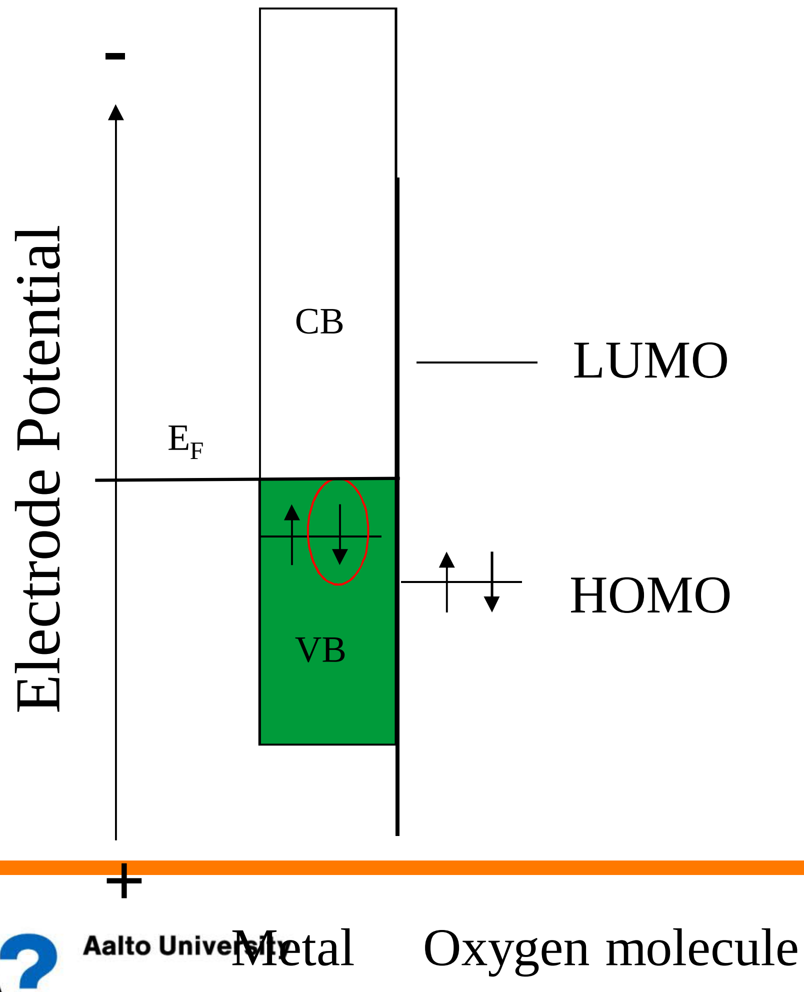



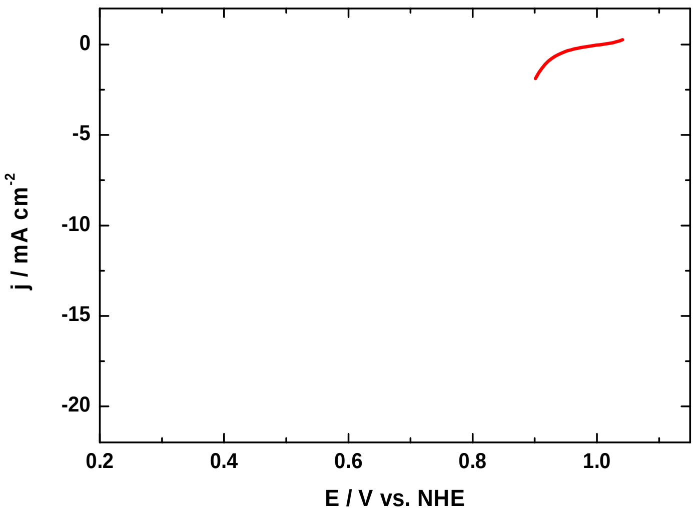
# Oxygen reduction – what will happend?



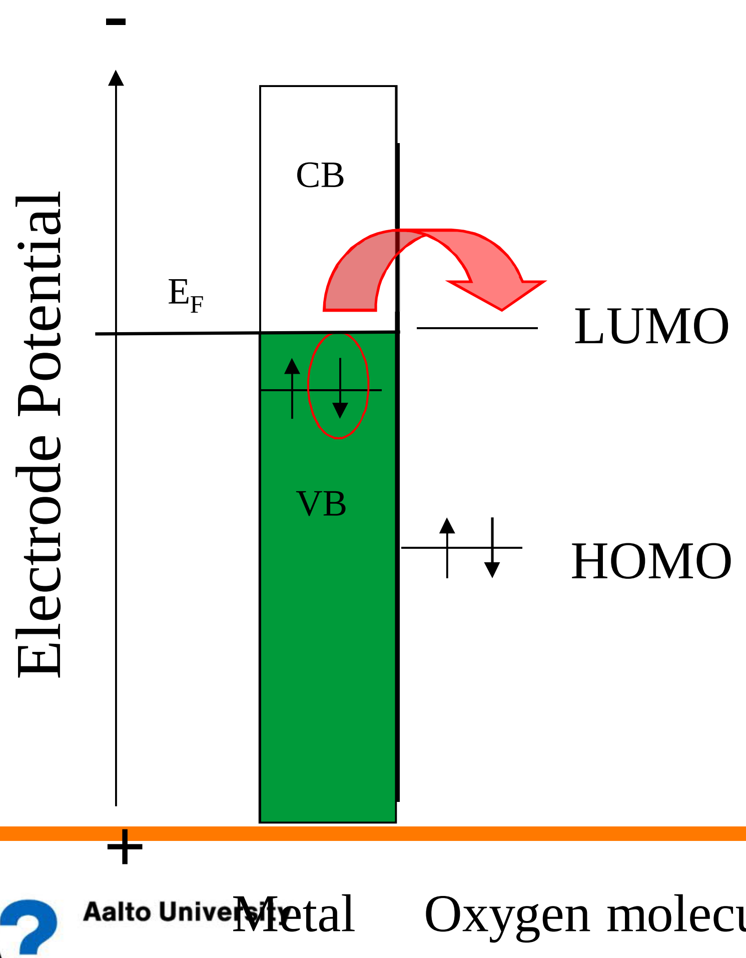



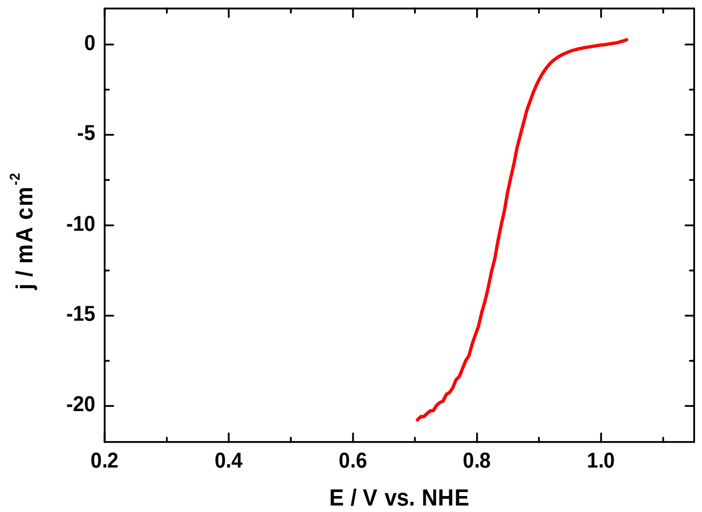
# Oxygen reduction



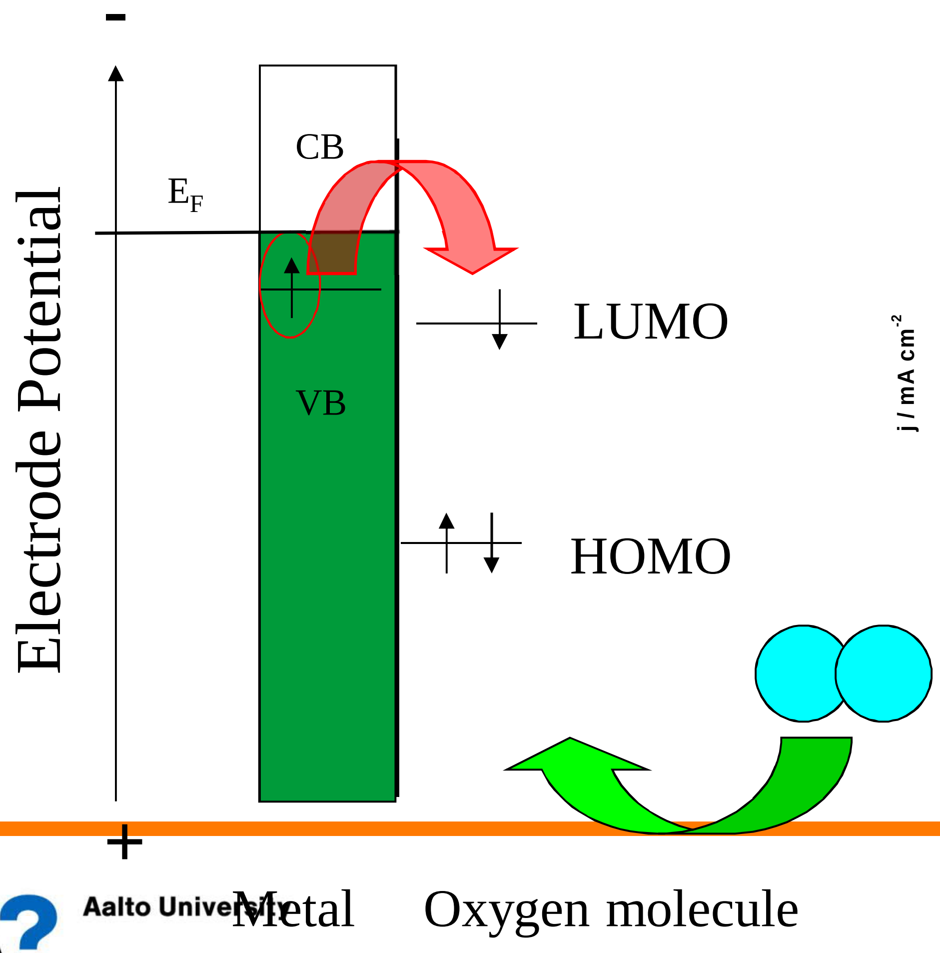



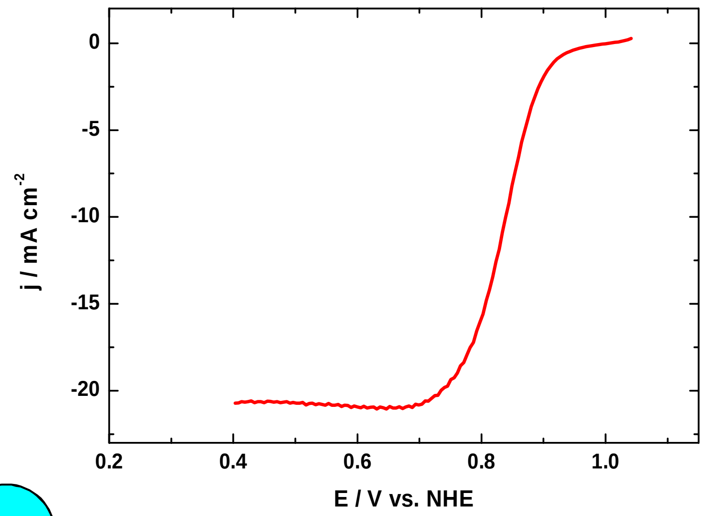
# Oxygen reduction



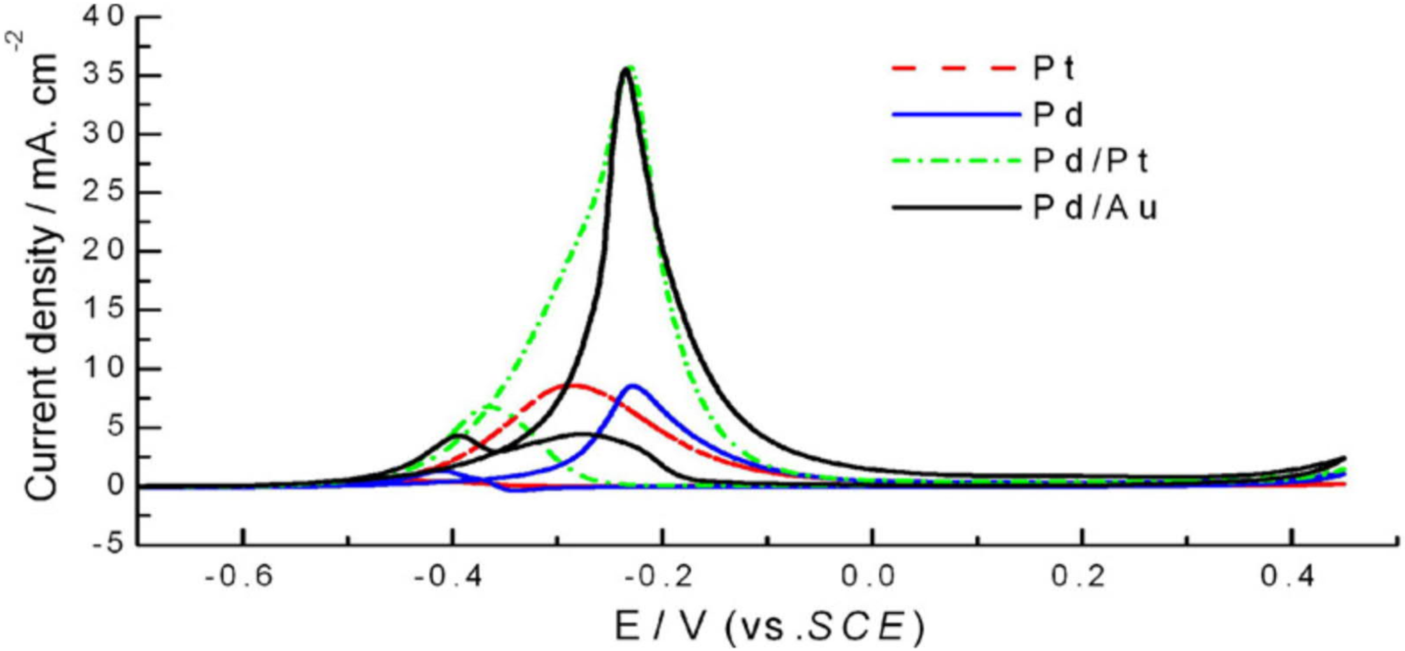
# Oxygen reduction



# Work function and it's relation to electrocatalyst

| | $\Phi$ /eV |
|---|---|
| Pd | 5.0 |
| Pt | 6.35 |

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EtOH oxidation in 0.1 M KOH solution on different electrode materials.

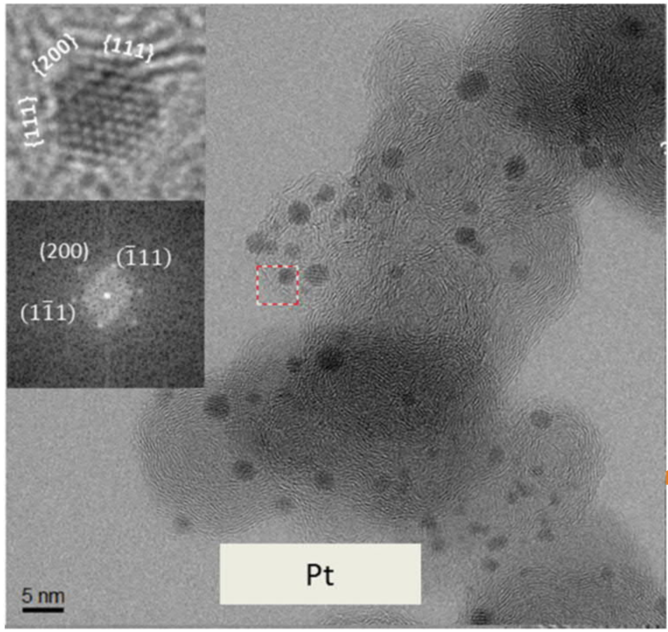
J. Zhang et al. Electrochem. Commun. 9 (2007) 1298.

# Surface orientation

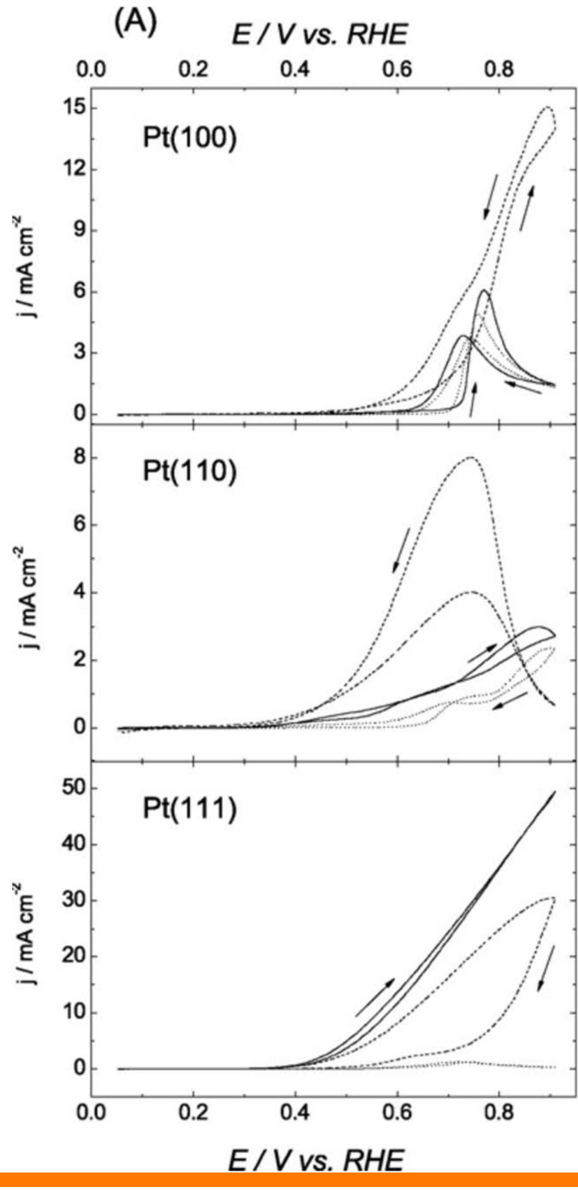
Crystalline structures

| | Φ (eV) |
|---|---|
| Pt(100) | 5.82[1] |
| Pt(110) | 5.85[2] |
| Pt(111) | 6.07[1] |


1) M. Salmerón et al. Phys. Ref. B 28 (1983) 6758.
2) D. R. Lide (Ed.), CRC Handbook of Chemistry and Physics, 80th ed., CRC Press, Boca Raton 1999/2000.


E. Sairanen et al. / Applied Catalysis B: Environmental 148–149 (2014) 11




Methanol (solid line), 2-Propanol (dashed line) and 50/50 mixture (thin line) oxidation in 0.1 M $HClO_4$ electrolyte on different surface orientations.

A. Santasalo et al. Electrochem. Acta 54 (2009) 6576.

# How to modify work function

- Alloying metals effects the work function of the electrode

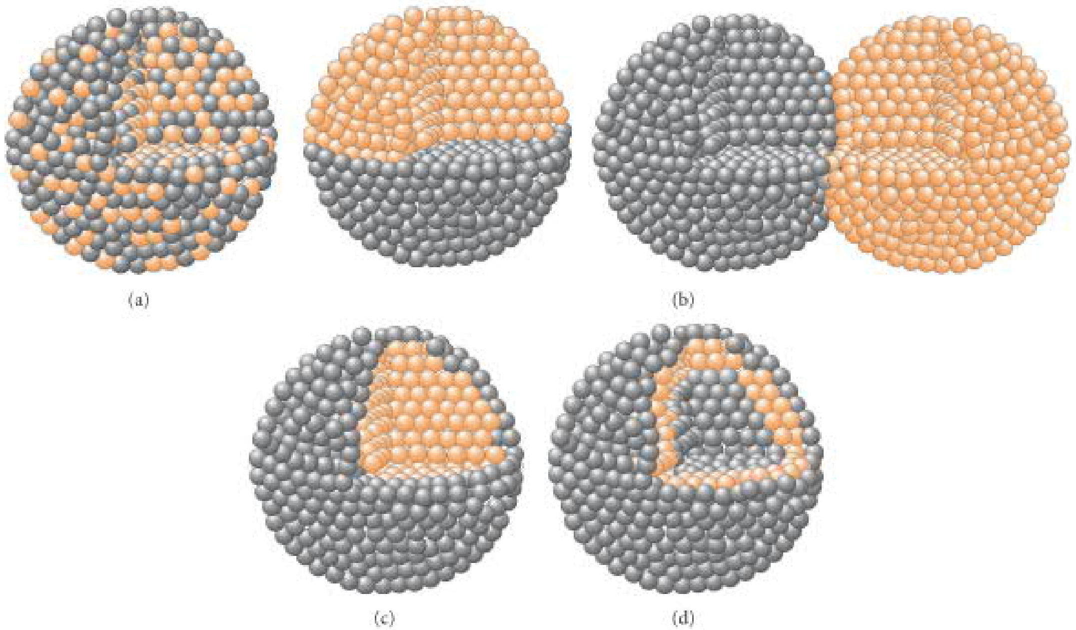
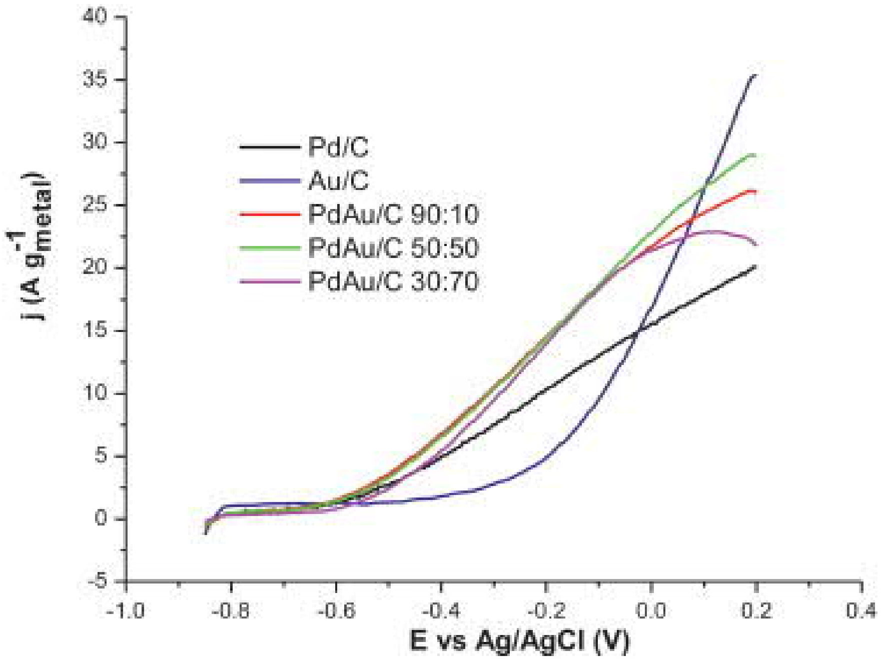


FIGURE 2: Schematic illustration of bimetallic NPs with different structures (a) alloy, (b) heterostructure, (c) core-shell, and (d) multishell structure.



Anna Zielińska-Jurek, Journal of Nanomaterials
Volume (2014), http://dx.doi.org/10.1155/2014/208920

# Different Catalysts in action




Ethanol oxidation in alkaline media (1 M KOH) on different catalyst. Au/C is gold nanoparticle catalyst on carbon support.

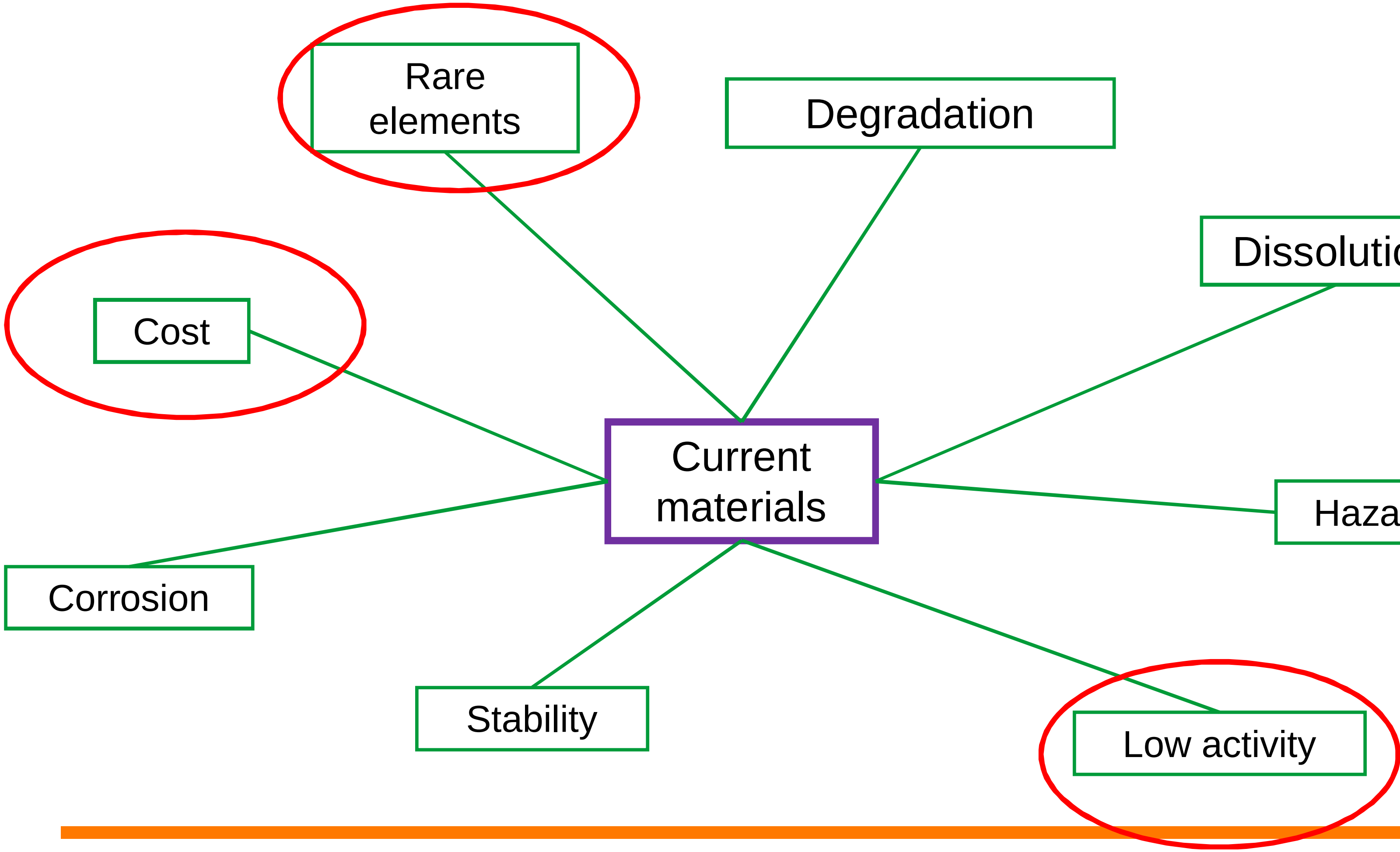
$$\chi^M = \frac{\Phi^M + \mu_e^M}{F}$$

What would be the best catalyst for this particular reaction?



A. Geraldes *et al.* Electrochimica Acta 111 (2013) 455.

# Challenges with materials

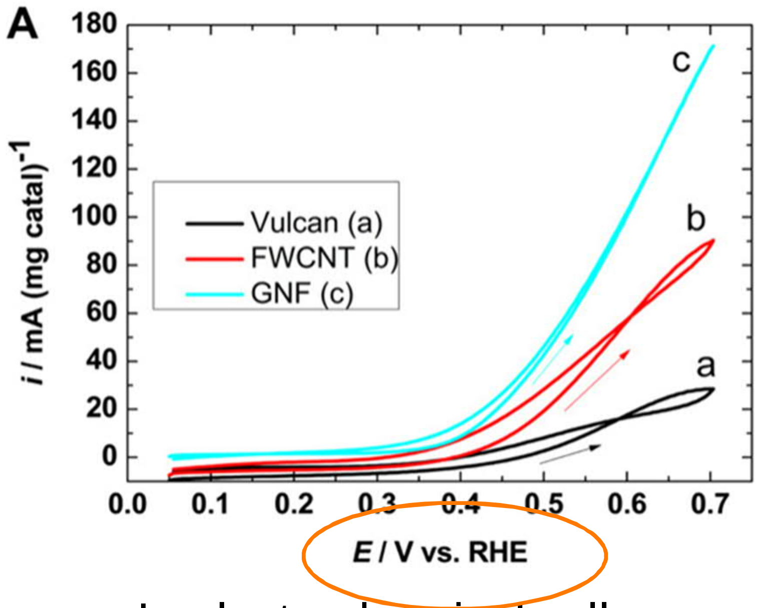


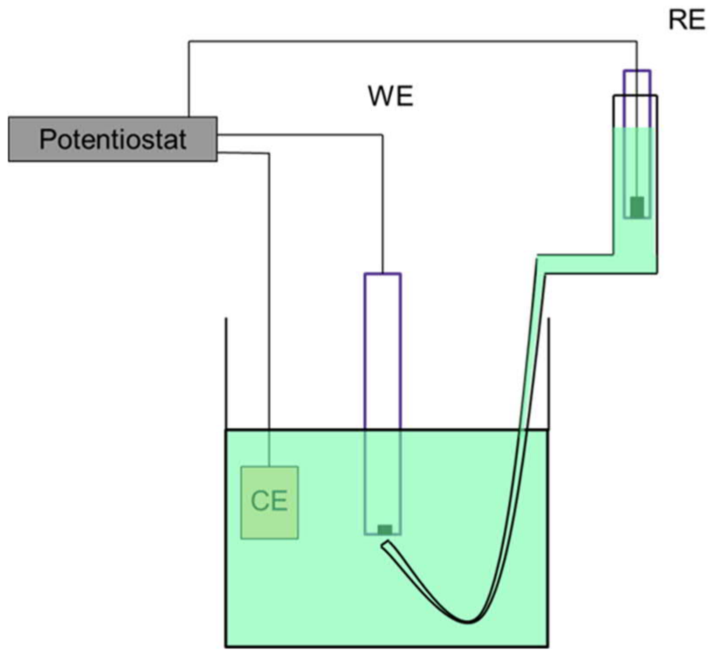



Development for active materials

# How to interpret catalyst material data?

3 Electrode set up:
To study individual electrode reaction




In electrochemical cell:
25 ºC
0.1 M HClO4 + 1 M MeOH

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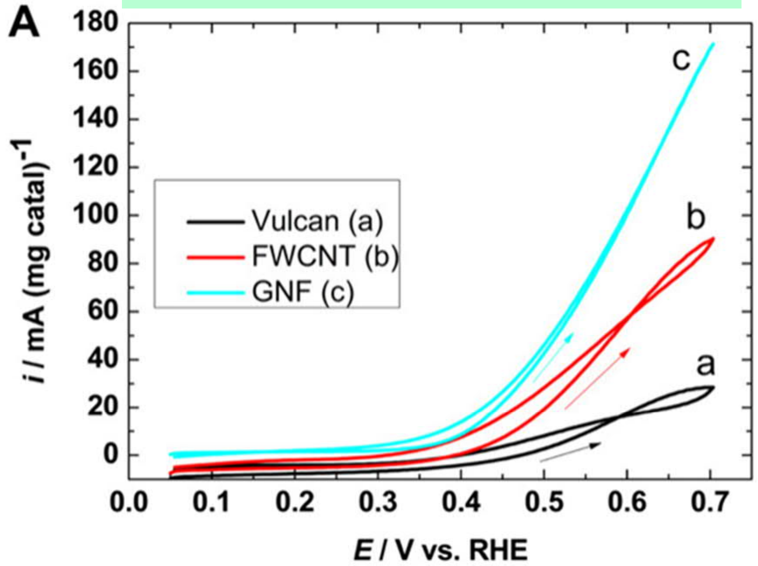
A. Santasalo-Aarnio et al. International Journal of Hydrogen Energy, 37 (2012) 3415-3424.

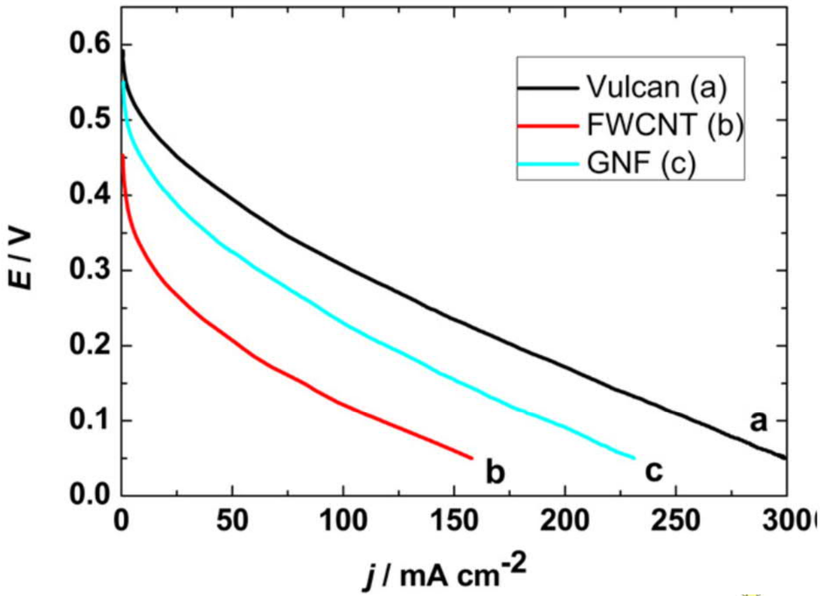
# How to interpret catalyst material data?

3 Electrode system
(anode reaction)

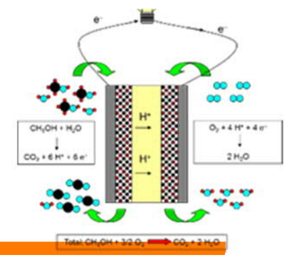



In electrochemical cell:
25 ºC
0.1 M HClO4 + 1 M MeOH

2 Electrode system
(anode + cathode)




Single cell fuel cell:
70 ºC
1 M MeOH





A. Santasalo-Aarnio et al. International Journal of Hydrogen Energy, 37 (2012) 3415-3424.

# Reflection


1. What was most interesting today?
2. I would have wanted to hear more on?

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# Task 2 instructions
# Task 3 groups and topics

# Task 2 – Pitch at 7.2.2019

Max. 3 min. -> Practice

***New material solution***

Slides (max. 4-5 slides):

1) Shortly your application
2) A material issue you are addressing
3) New material solution
4) Why should your idea be funded?

+

Slide with references (this does not need to be part of the pitch but is part of the submission)



One person will pitch and that person is selected at class.
- > All students need to be ready to pitch!

# Task 2 – Evaluation

***New material solution***

Innovation potential max .8 p.

Credibility and the need for this solution max. 7 p.

<u>Delivering the message max. 5 p.</u>

Total 20 p.

The slide must have reference slide in the end, indicating what the idea is based on.

# Task 3 group forming

- One member in the group will stay with the topic as the new team leader (the group can decide who will stay)
- Other team members will list 3 favorable options for the next team topics

- We will prepare the teams for the next time, team leaders will gather the team next ween
- Flip still is related to the old topic (task 2)

# Groups and Topics: Task 3

**Off-Shore Wind**
- Expert

**Thermal Storage**
-Expert

**Flow Battery**
- Expert

**Solar PV**
- Expert

**Solid Oxide Fuel Cell**
- Jarkko

**Concentrated Solar Power**
- Lillian

**Marine**
- Expert



**Who are the team experts?**

# Task 3 – Eco-design
## Presented at 28.2 14-17

- Eco-design is material design taking into account the recyclability of the application at end-of-life
- This can be new material solution, new design, reselection of materials
- But also … new concept, new business opportunities

- You need to first know the current status of your application

# Task 1 results

# Off shore - Wind

Group A

Result 1: 262 days

Result 2: 155 days

- Radius
- Peak performance used

….Further iteration

- Group B

Result 1: 10 month ~300 days

Result 2: 11 months ~330 days

- With recycling (Steel recycling energy intensive)

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# Next workshop V

# Next workshop V

- New Material Solutions (Pitching)

- New teams and topics announced
- What are the materials of those application
- How rare are the materials used (can they be scaled up?)

  -> “Light Poster”

- Theory: The Recycling Challenge

# Flip report IV:

**1)** **“**Addressing the terawatt challenge: scalability in the supply of chemical elements for renewable energy”
P.C.K. Vesborg, RSC Adv. 2 (2012) 7933-7947.
**ALL STUDENTS**
**MyCoursese – Materials – Material Development**

**2) News paper clip: “Metal material mining”**
Preferable in your application (if not found any on course topic)
(any country, any language)

**3) Journal Paper: your application that can help you with Task 2**
New Material Solutions that other have been presenting

# Flip reports – peer review

- Student number to your task

- Select one flip that is from other topic than your own
- Read and evaluate the report (15 min.)
- Write at least 2 sentence of feedback
  – What was good/interesting or/and what could be improved
- Grade
  – 3 p. Excellent work
  – 2 p. Good work
  – 1 p. Some parts missing/ Unclear text
  – 0 p. No submission

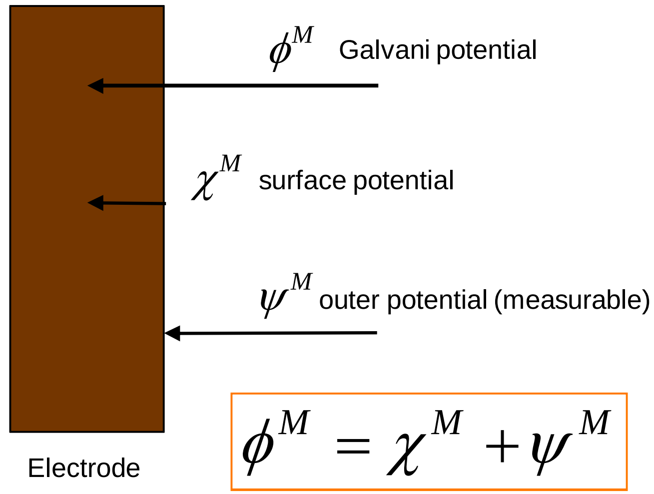
# Additional material
# Electrochemical potential

# Electrochemical potential

Electrochemical potential (in general)

$$\tilde{\mu}_i^a = \mu_i^a + z_i F \phi^a$$

For an electron in a metal phase?




$$\phi^M = \chi^M + \psi^M$$

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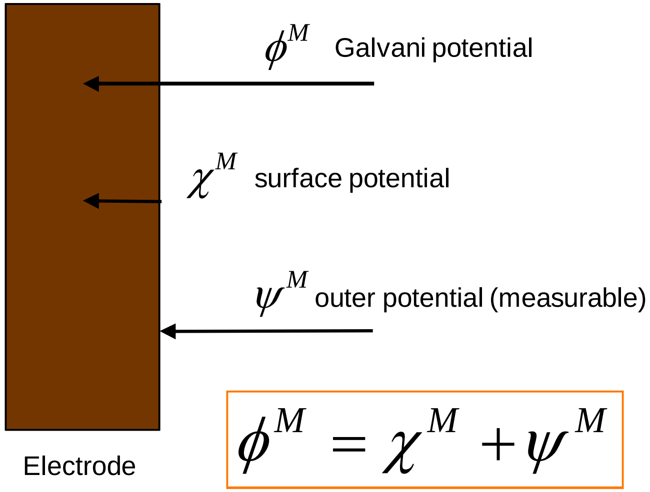


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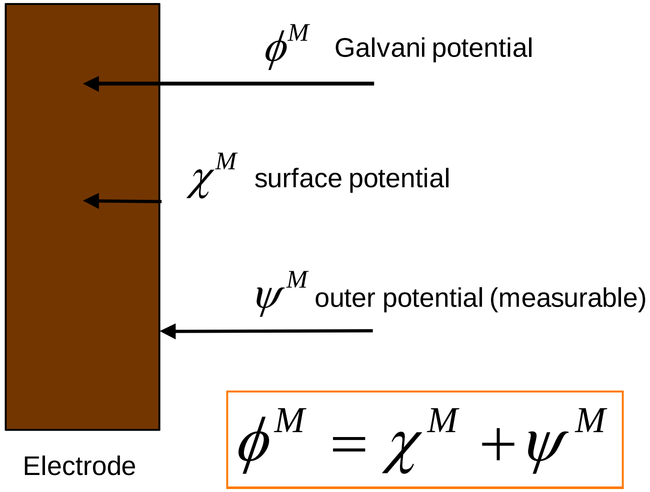
Surface and outer potential?

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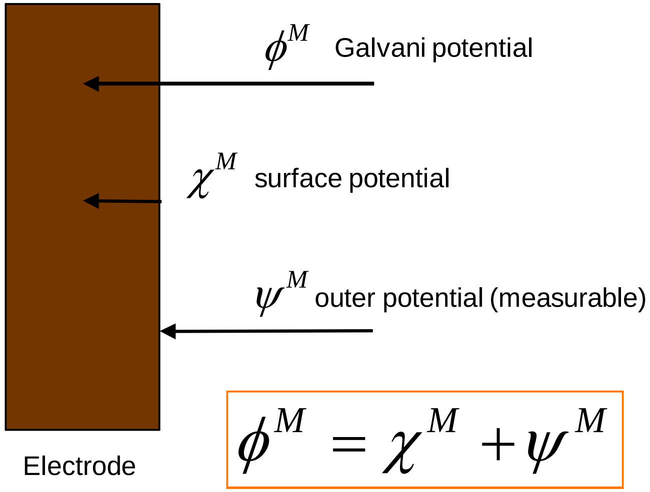


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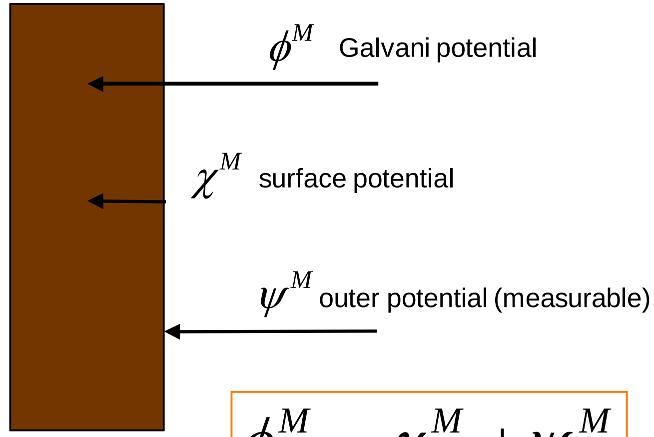
If the electrode is not charged, outer potential of the metal is 0



Electrode

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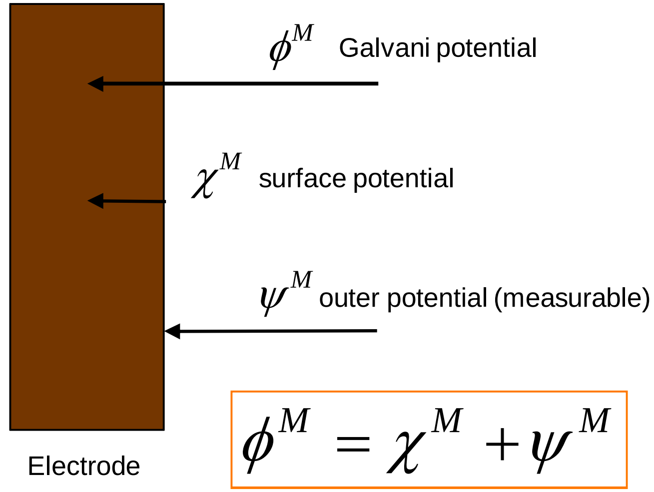
# Electrochemical potential

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